LOGINID:SSSPTA1623PAZ

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'HOME' AT 07:10:27 ON 27 JUN 2003
FILE 'HOME' ENTERED AT 07:10:27 ON 27 JUN 2003

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.05	1.05

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.05	1.05

FILE 'STNGUIDE' ENTERED AT 07:10:37 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.06	1.11

FILE 'HOME' ENTERED AT 07:10:40 ON 27 JUN 2003

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	1.32

FILE 'STNGUIDE' ENTERED AT 07:10:52 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.12	1.44

FILE 'HOME' ENTERED AT 07:12:21 ON 27 JUN 2003

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	1.65

FILE 'STNGUIDE' ENTERED AT 07:12:34 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 20, 2003 (20030620/UP).

```
=> FIL HOME
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.06       1.71

FILE 'HOME' ENTERED AT 07:13:22 ON 27 JUN 2003

=> logoff hold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.84       2.55

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:15:28 ON 27 JUN 2003

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSPTA1623PAZ

PASSWORD:
LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid.
You either typed them incorrectly, or line noise may
have corrupted them.

Do you wish to retry the logon?
Enter choice (y/N):

Connecting via Winsock to STN

LOGINID:

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSPTA1623PAZ

PASSWORD:
LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid.
You either typed them incorrectly, or line noise may
have corrupted them.

Do you wish to retry the logon?
Enter choice (y/N):

Connecting via Winsock to STN
```

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Jun 03	New e-mail delivery for search results now available
NEWS 4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 7	Sep 03	JAPIO has been reloaded and enhanced
NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11	Oct 24	BEILSTEIN adds new search fields
NEWS 12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13	Nov 18	DKILIT has been renamed APOLLIT
NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN
NEWS 16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 20	EVENTLINE will be removed from STN
NEWS 28	Mar 24	PATDPAFULL now available on STN
NEWS 29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 30	Apr 11	Display formats in DGENE enhanced
NEWS 31	Apr 14	MEDLINE Reload
NEWS 32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 33	Jun 13	Indexing from 1947 to 1956 added to records in CA/CAPLUS
NEWS 34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 35	Apr 28	RDISCLOSURE now available on STN
NEWS 36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS 38	May 15	Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39	May 16	CHEMREACT will be removed from STN
NEWS 40	May 19	Simultaneous left and right truncation added to WSCA
NEWS 41	May 19	RAPRA enhanced with new search field, simultaneous left and right truncation
NEWS 42	Jun 06	Simultaneous left and right truncation added to CBNB
NEWS 43	Jun 06	PASCAL enhanced with additional data
NEWS 44	Jun 20	2003 edition of the FSTA Thesaurus is now available
NEWS 45	Jun 25	HSDB has been reloaded

```
 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:29:25 ON 27 JUN 2003

=> logoff hold
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.84       0.84

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:31:42 ON 27 JUN 2003

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'HOME' AT 08:44:40 ON 27 JUN 2003
FILE 'HOME' ENTERED AT 08:44:40 ON 27 JUN 2003

COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.84       0.84

=> file mreg
'MREG' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'HOME'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available.  If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       1.05       1.05

FILE 'REGISTRY' ENTERED AT 08:45:01 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
```

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10075845 generic six.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam
SAMPLE SEARCH INITIATED 08:45:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

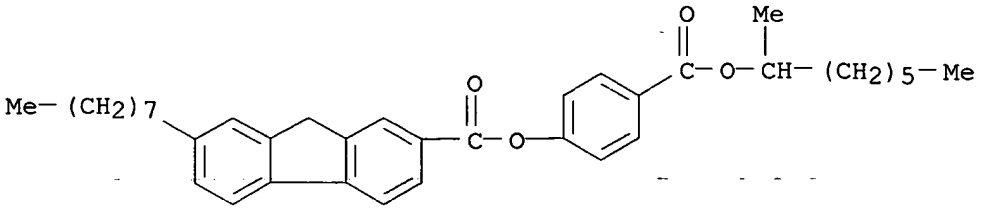
32.4% PROCESSED 1000 ITERATIONS 3 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 58448 TO 65112
PROJECTED ANSWERS: 3 TO 367

L2 3 SEA SSS SAM L1

=> d scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-octyl-, 4-[[(1-methylheptyl)oxy]carbonyl]phenyl ester (9CI)
MF C37 H46 O4



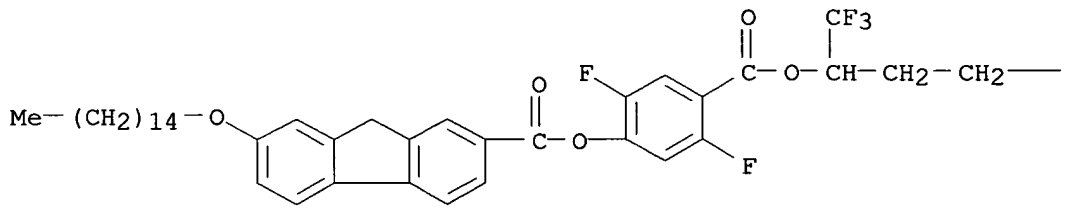
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):lofgoff hold
'LOFGOFF HOLD' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(pentadecyloxy)-, 4-[[[4-ethyl-1-(trifluoromethyl)hexyl]oxy]carbonyl]-2,5-difluorophenyl ester (9CI)
MF C45 H57 F5 O5

PAGE 1-A

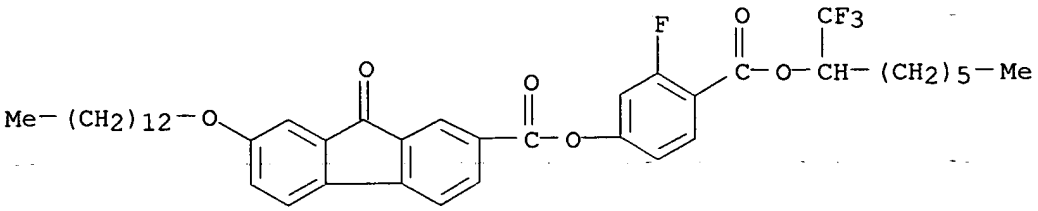


PAGE 1-B

— $CHEt_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 9-oxo-7-(tridecyloxy)-, 3-fluoro-4-[[[1-(trifluoromethyl)heptyl]oxy]carbonyl]phenyl ester (9CI)
MF C42 H50 F4 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.80	1.85

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:46:27 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 08:48:38 ON 27 JUN 2003
FILE 'REGISTRY' ENTERED AT 08:48:38 ON 27 JUN 2003
COPYRIGHT (C) 2003 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.80	1.85

=>
Uploading 10075845 generic six.str

L3 STRUCTURE UPLOADED

=> d l13
L13 NOT FOUND
The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> d l3
L3 HAS NO ANSWERS
L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

```
=> search l3 sss sam
SAMPLE SEARCH INITIATED 08:49:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3089 TO ITERATE

 32.4% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        58448 TO    65112
PROJECTED ANSWERS:               0 TO        0

L4            0 SEA SSS SAM L3

=> search l3 sss full
FULL SEARCH INITIATED 08:50:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  62195 TO ITERATE

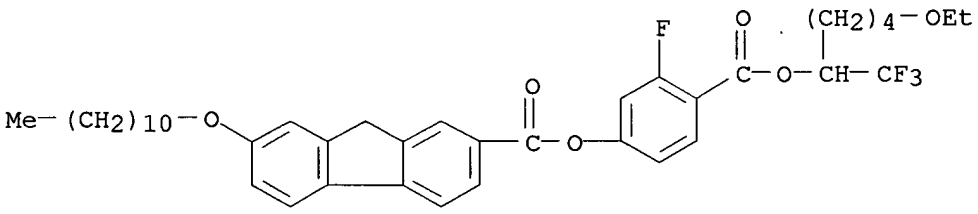
100.0% PROCESSED   62195 ITERATIONS                              137 ANSWERS
SEARCH TIME: 00.00.03

L5          137 SEA SSS FUL L3

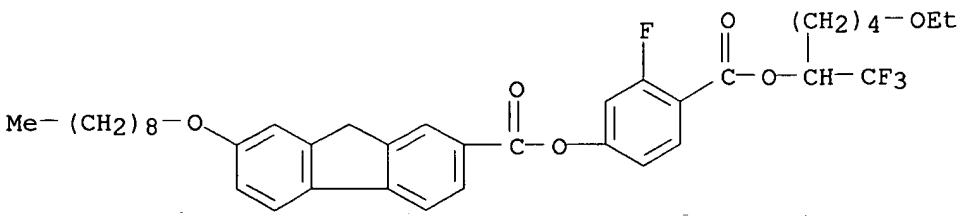
=> d scan

L5   137 ANSWERS   REGISTRY  COPYRIGHT 2003 ACS
IN   9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-
     trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with
     4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl
     7-(undecyloxy)-9H-fluorene-2-carboxylate, 1-methylheptyl
     4-[6-(4-hexylphenyl)-3-pyridinyl]benzoate, 4-[[(1-
     methylheptyl)oxy]carbonyl]phenyl 4'-(octyloxy)[1,1'-biphenyl]-4-
     carboxylate and 4-[[(1-methylheptyl)oxy]carbonyl]phenyl
     4-[[4-(undecyloxy)benzoyl]oxy]benzoate (9CI)
MF   C40 H52 O7 . C40 H48 F4 O6 . C38 H44 F4 O6 . C36 H46 O5 . C32 H41 N O2
CI   MXS

     CM   1
```

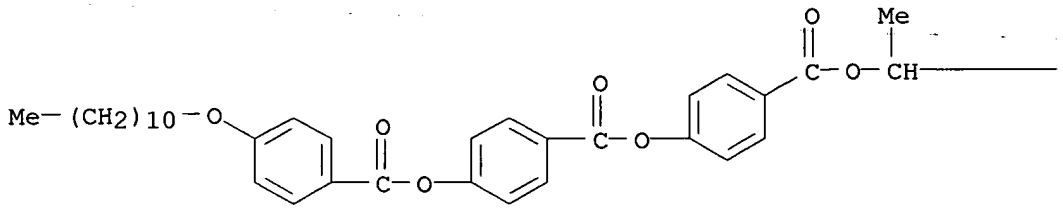



```
     CM   2
```



CM 3

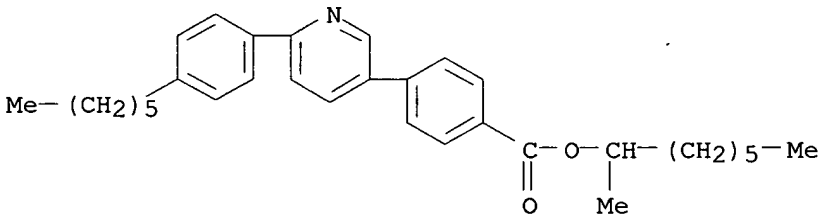
PAGE 1-A



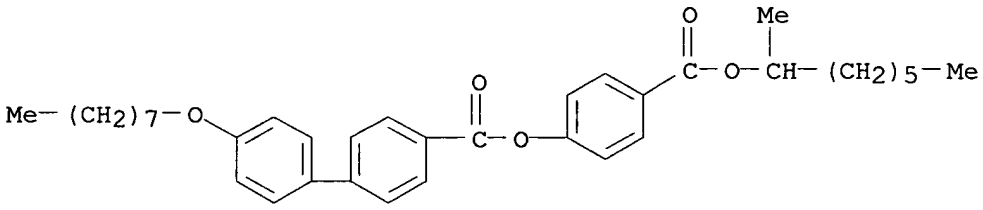
PAGE 1-B

— $(CH_2)_5$ — Me

CM 4



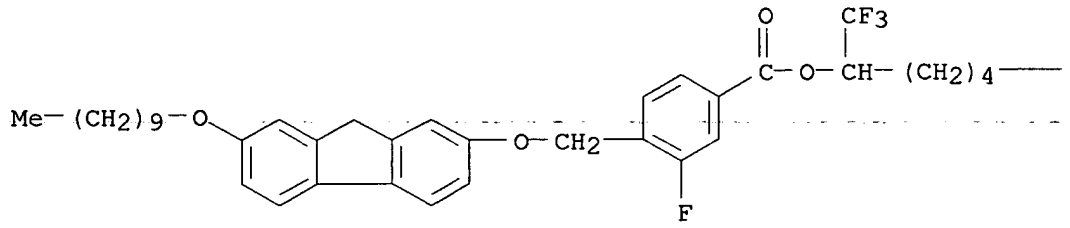
CM 5



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[[7-(decyloxy)-9H-fluoren-2-yl]oxy]methyl]-3-fluoro-, 5-ethoxy-1-(trifluoromethyl)pentyl ester (9CI)
MF C39 H48 F4 O5

PAGE 1-A

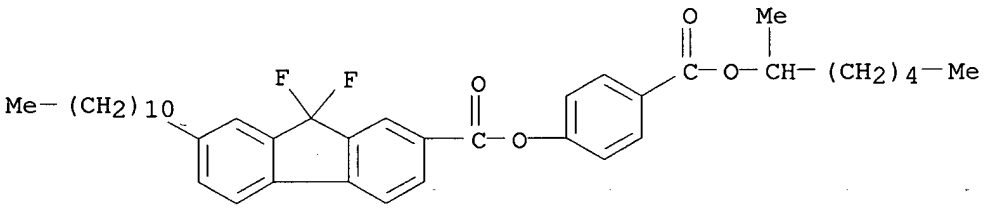


PAGE 1-B

—OEt

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

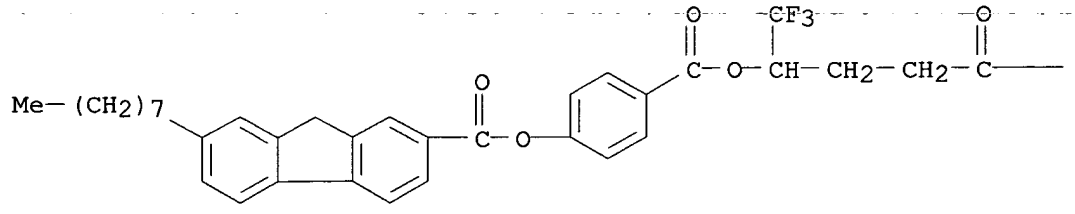
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 9,9-difluoro-7-undecyl-, 4-[[(1-methylhexyl)oxy]carbonyl]phenyl ester (9CI)
MF C39 H48 F2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-octyl-, 4-[[4-butoxy-4-oxo-1-(trifluoromethyl)butoxy]carbonyl]phenyl ester (9CI)
MF C38 H43 F3 O6

PAGE 1-A



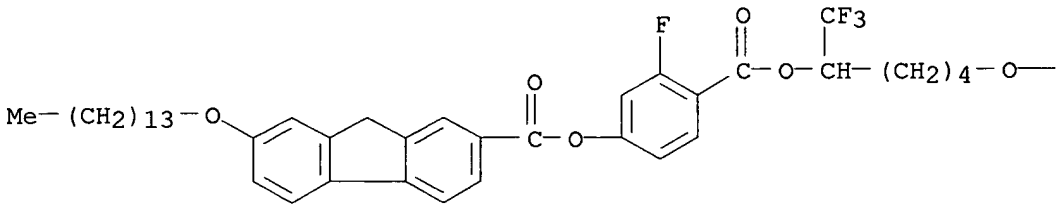
PAGE 1-B

—OBu-n

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(tetradecyloxy)-, 3-fluoro-4-[[2,2,2-trifluoro-1-[4-(2,2,2-trifluoroethoxy)butyl]ethoxy]carbonyl]phenyl ester (9CI)
MF C43 H51 F7 O6

PAGE 1-A

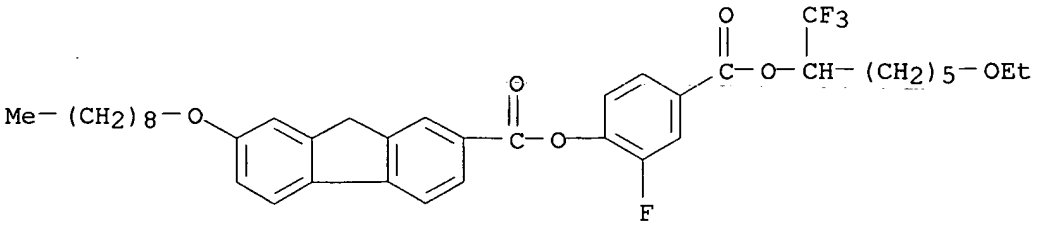


PAGE 1-B

—CH2—CF3

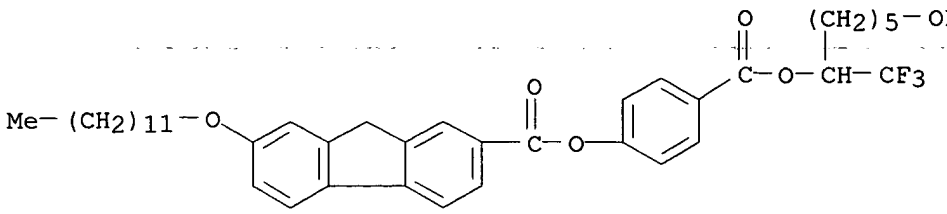
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[[6-ethoxy-1-(trifluoromethyl)hexyl]oxy]carbonyl]-2-fluorophenyl ester (9CI)
MF C39 H46 F4 O6



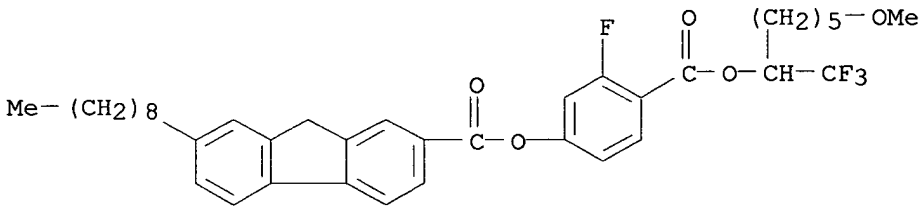
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[[6-ethoxy-1-(trifluoromethyl)hexyl]oxy]carbonyl]phenyl ester (9CI)
MF C42 H53 F3 O6



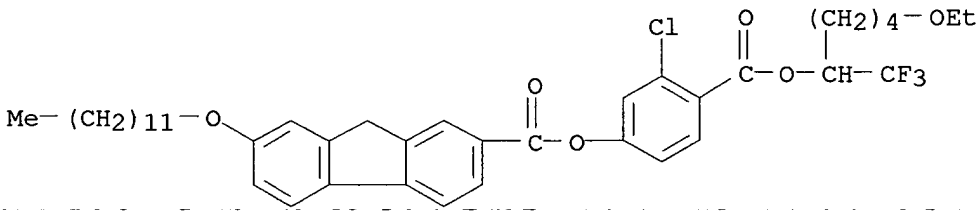
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-nonyl-, 3-fluoro-4-[[2,2,2-trifluoro-1-(5-methoxypentyl)ethoxy]carbonyl]phenyl ester (9CI)
MF C38 H44 F4 O5



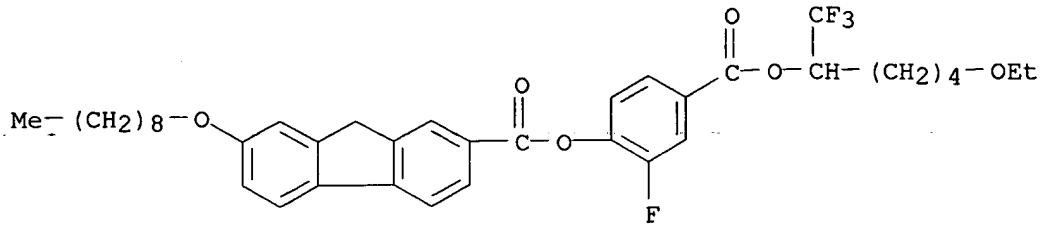
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 3-chloro-4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]phenyl ester (9CI)
MF C41 H50 Cl F3 O6



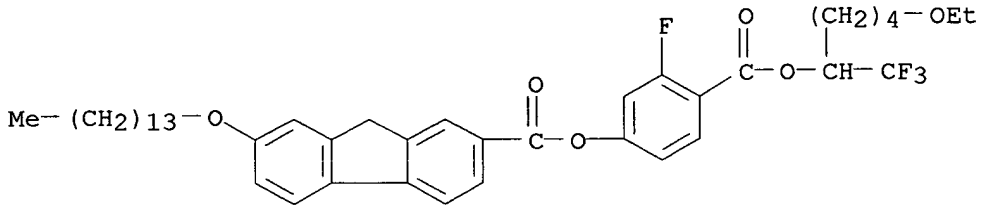
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-2-fluorophenyl ester (9CI)
MF C38 H44 F4 O6



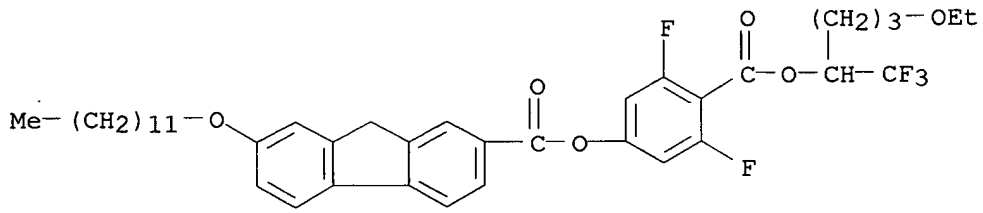
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(tetradecyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester (9CI)
MF C43 H54 F4 O6



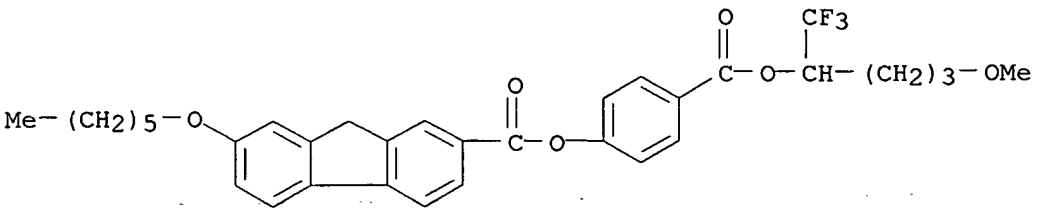
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[4-ethoxy-1-(trifluoromethyl)butoxy]carbonyl]-3,5-difluorophenyl ester (9CI)
MF C40 H47 F5 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

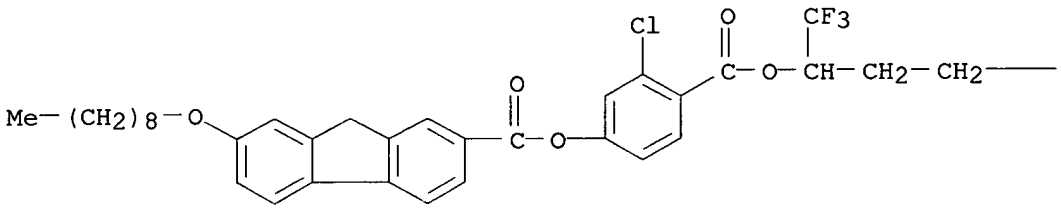
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(hexyloxy)-, 4-[[4-methoxy-1-(trifluoromethyl)butoxy]carbonyl]phenyl ester (9CI)
MF C33 H35 F3 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 3-chloro-4-[[3-ethoxy-1-(trifluoromethyl)propoxy]carbonyl]phenyl ester (9CI)
MF C36 H40 Cl F3 O6

PAGE 1-A

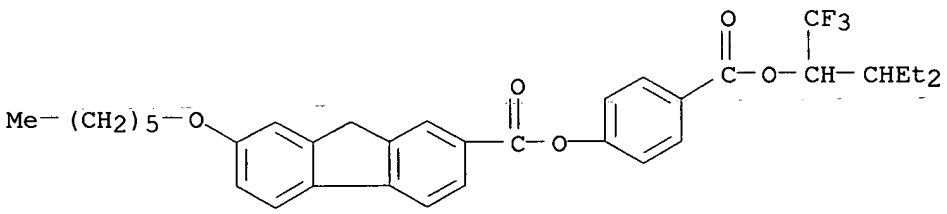


PAGE 1-B

—OEt

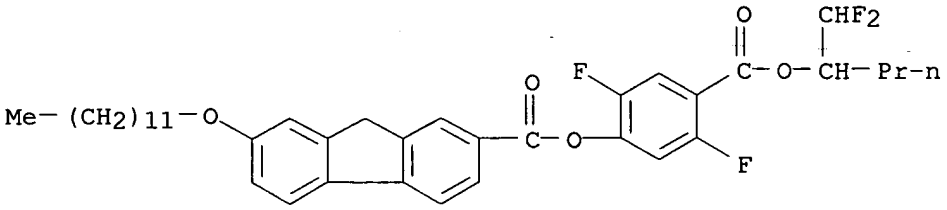
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(hexyloxy)-, 4-[[2-ethyl-1-(trifluoromethyl)butoxy]carbonyl]phenyl ester (9CI)
MF C34 H37 F3 O5



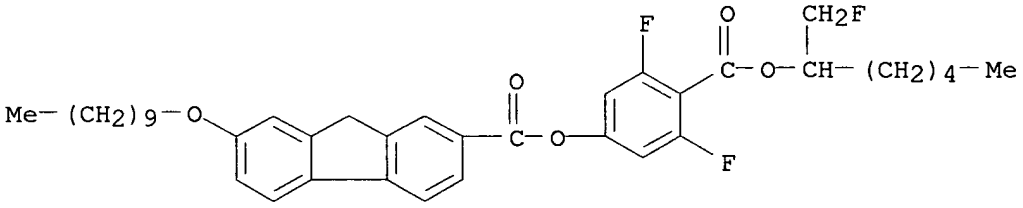
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[1-(difluoromethyl)butoxy]carbonyl]-2,5-difluorophenyl ester (9CI)
MF C38 H44 F4 O5



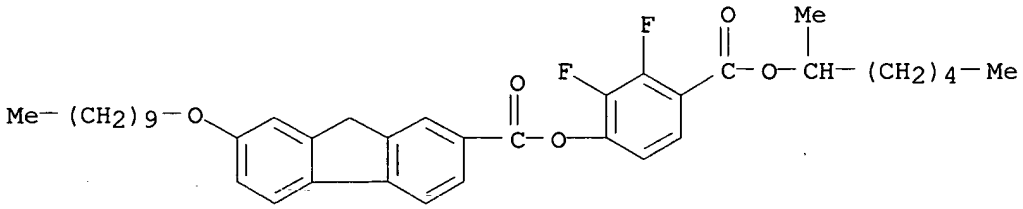
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(decyloxy)-, 3,5-difluoro-4-[[[1-(fluoromethyl)hexyl]oxy]carbonyl]phenyl ester (9CI)
MF C38 H45 F3 O5



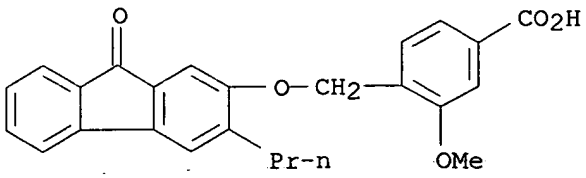
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(decyloxy)-, 2,3-difluoro-4-[[(1-methylhexyl)oxy]carbonyl]phenyl ester (9CI)
MF C38 H46 F2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

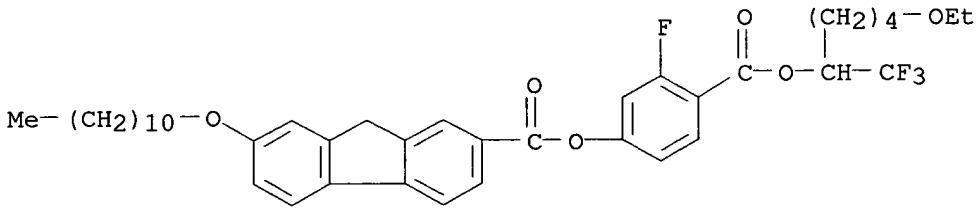
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-methoxy-4-[[(9-oxo-3-propyl-9H-fluoren-2-yl)oxy]methyl]- (9CI)
MF C25 H22 O5



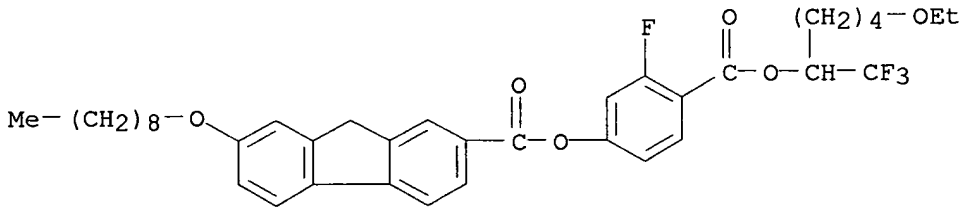
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl 7-(undecyloxy)-9H-fluorene-2-carboxylate, 4-[[(1-methylheptyl)oxy]carbonyl]phenyl 4-(octyloxy)benzoate, 4-[[(1-methylheptyl)oxy]carbonyl]phenyl 4'-(octyloxy)[1,1'-biphenyl]-4-carboxylate and 4-[[(1-methylheptyl)oxy]carbonyl]phenyl 4-[[4-(undecyloxy)benzoyl]oxy]benzoate (9CI)
MF C40 H52 O7 . C40 H48 F4 O6 . C38 H44 F4 O6 . C36 H46 O5 . C30 H42 O5
CI MXS

CM 1



CM 2



CM 3

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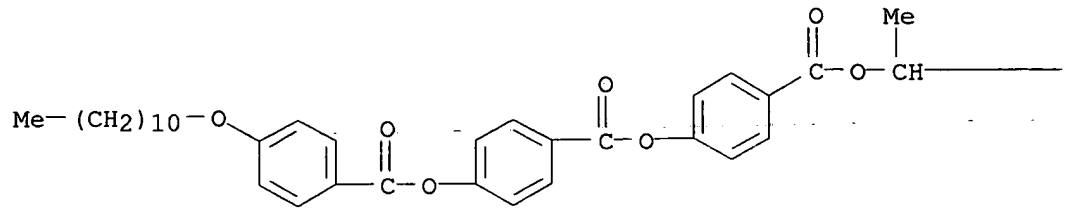

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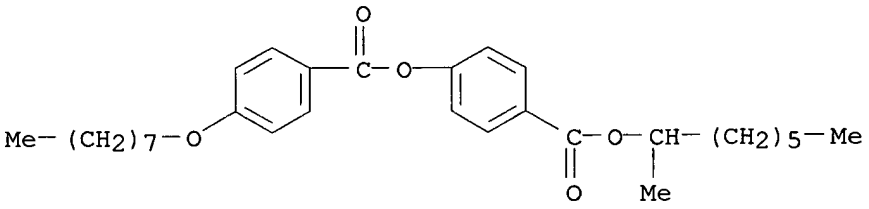
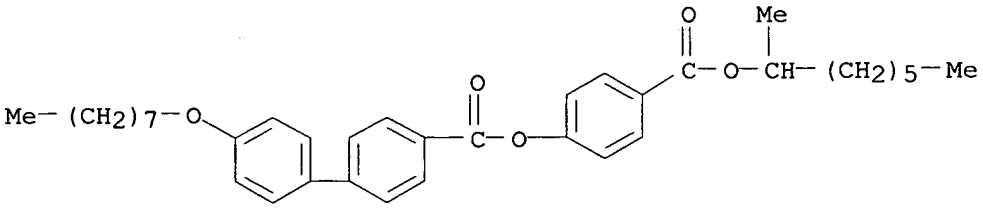
— $(CH_2)_5$ — Me

CM 4

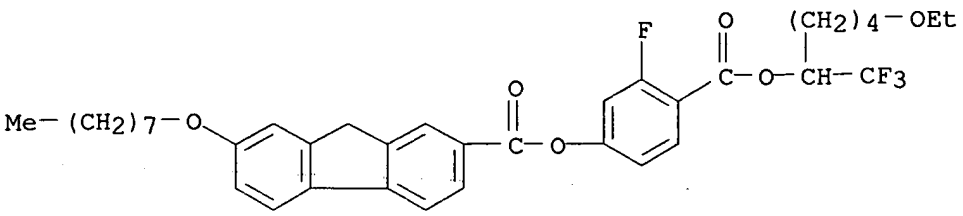


CM 5

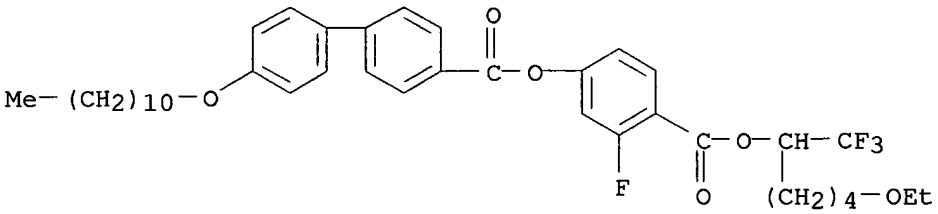


L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(octyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with 4-[[[5-ethoxy-1-(trifluoromethyl)pentyl]oxy]carbonyl]-3-fluorophenyl 4'-(undecyloxy)[1,1'-biphenyl]-4-carboxylate (9CI)
MF C39 H48 F4 O6 . C37 H42 F4 O6
CI MXS

CM 1



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=>
Uploading 10075845 generic six.str

L6 STRUCTURE UPLOADED

=> d l6
L6 HAS NO ANSWERS
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> search l6 sss sam
SAMPLE SEARCH INITIATED 08:54:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 58448 TO 65112
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

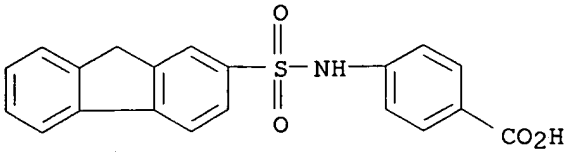
=> search l6 sss full
FULL SEARCH INITIATED 08:54:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62195 TO ITERATE

100.0% PROCESSED 62195 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.03

L8 3 SEA SSS FUL L6

=> d scan

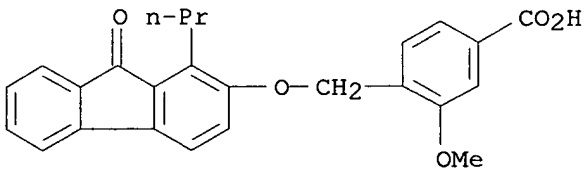
L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(9H-fluoren-2-ylsulfonyl)amino]- (9CI)
MF C20 H15 N O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

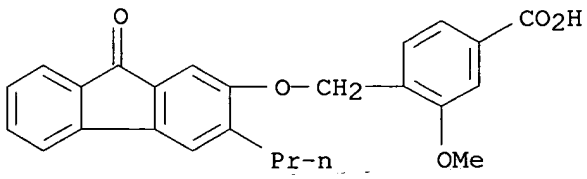
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-methoxy-4-[[(9-oxo-1-propyl-9H-fluoren-2-yl)oxy]methyl]-
(9CI)
MF C25 H22 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-methoxy-4-[[(9-oxo-3-propyl-9H-fluoren-2-yl)oxy]methyl]-
(9CI)
MF C25 H22 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

```
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       301.90     302.95

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:57:09 ON 27 JUN 2003

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 09:05:09 ON 27 JUN 2003
FILE 'REGISTRY' ENTERED AT 09:05:09 ON 27 JUN 2003
COPYRIGHT (C) 2003 American Chemical Society (ACS)

COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       301.90     302.95

=>
Uploading 10075845 generic six crrct.str

L9      STRUCTURE UPLOADED

=> d l9
L9 HAS NO ANSWERS
L9              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> search l9 sss sam
SAMPLE SEARCH INITIATED 09:06:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3229 TO ITERATE

 31.0% PROCESSED    1000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        61173 TO    67987
PROJECTED ANSWERS:               0 TO        0

L10           0 SEA SSS SAM L9

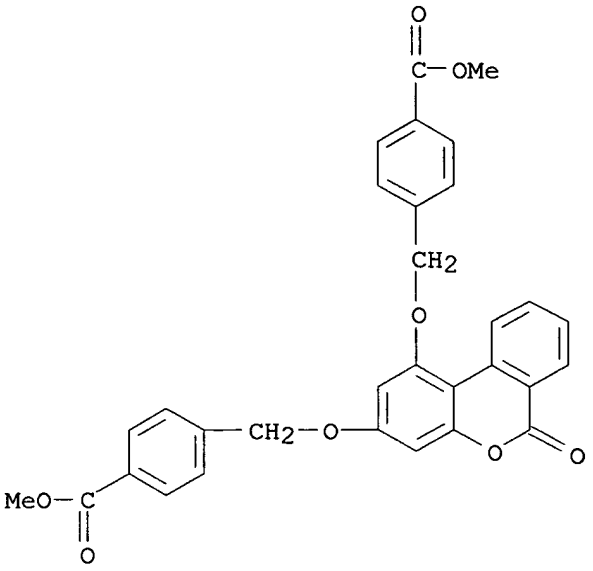
=> search l9 sss full
FULL SEARCH INITIATED 09:06:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  65007 TO ITERATE

100.0% PROCESSED   65007 ITERATIONS                            6 ANSWERS
SEARCH TIME: 00.00.03

L11           6 SEA SSS FUL L9
```

=> d scan

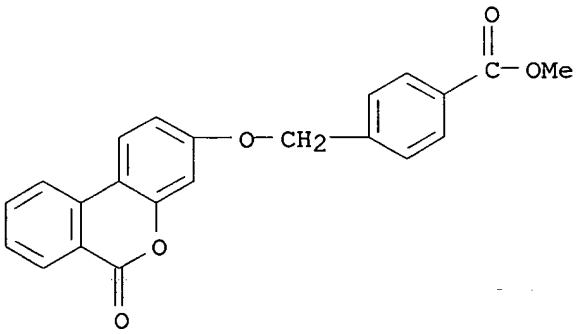
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4,4'-[(6-oxo-6H-dibenzo[b,d]pyran-1,3-diyl)bis(oxymethylene)]bis-, dimethyl ester (9CI)
MF C31 H24 O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):6

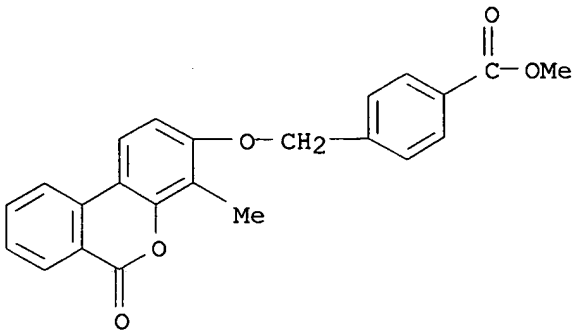
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester (9CI)
MF C22 H16 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

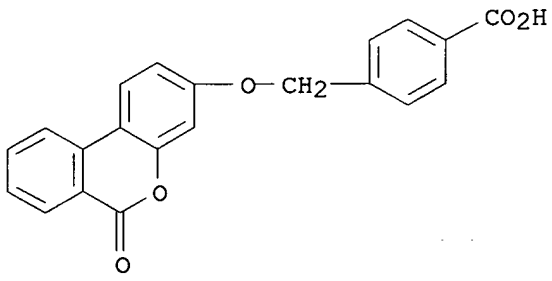
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-,

methyl ester (9CI)
MF C23 H18 O5



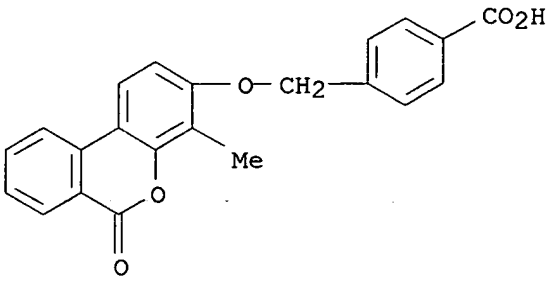
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]- (9CI)
MF C21 H14 O5



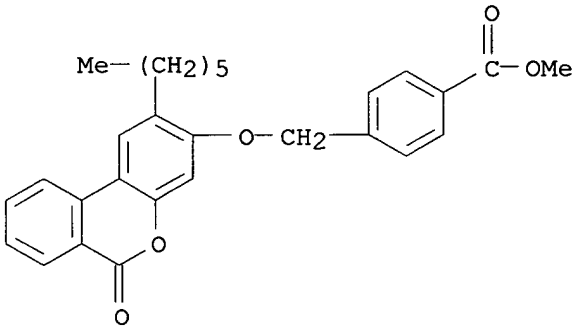
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
(9CI)
MF C22 H16 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester (9CI)
MF C28 H28 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	452.05	453.10

FILE 'CAPLUS' ENTERED AT 09:09:01 ON 27 JUN 2003
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 16
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:09:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 58448 TO 65112
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L6

L13 0 L12

=> l11
L14 0 L11

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.42 454.34

FILE 'CAPLUS' ENTERED AT 09:09:41 ON 27 JUN 2003
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26

FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l11
L15 0 L11

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	454.76

FILE 'REGISTRY' ENTERED AT 09:10:33 ON 27 JUN 2003
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STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> search l9 sss full
FULL SEARCH INITIATED 09:10:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 65007 TO ITERATE

100.0% PROCESSED 65007 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.03

L16 6 SEA SSS FUL L9

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.15	602.91

FILE 'CAPLUS' ENTERED AT 09:11:00 ON 27 JUN 2003
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l16
L17 0 L16

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	603.33

FILE 'REGISTRY' ENTERED AT 09:11:36 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> e Benzoic acid, 4-(((6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy)methyl)-/cn

E1	1	BENZOIC ACID, 4-(((6-O-ACETYL-2,3,4-TRIS-O-(PHENYLMETHYL)-.ALPHA.-D-MANNOPYRANOSYL)OXY)METHYL)-3-NITRO-, METHYL ESTER/CN
E2	1	BENZOIC ACID, 4-(((6-OXO-2,4-CYCLOHEXADIEN-1-YLIDENE)METHYL)AMINO)-, METHYL ESTER/CN
E3	0 -->	BENZOIC ACID, 4-(((6-OXO-6H-DIBENZOB,DPYRAN-3-YL)OXY)METHYL)-/CN
E4	1	BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHYL)-/CN
E5	1	BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHYL)-, METHYL ESTER/CN
E6	1	BENZOIC ACID, 4-(((6-QUINOXALINYLAMINO)THIOXOMETHYL)AMINO)-, METHYL ESTER/CN
E7	1	BENZOIC ACID, 4-(((6R)-6-(((2S)-2-(ACETYLAMINO)-1-OXO-3-(4-(PHOSPHONOOXY)PHENYL)PROPYL)AMINO)TETRAHYDRO-5-OXO-1,4-THIAZEPIN-4(5H)-YL)METHYL)-, 1-METHYL ESTER/CN
E8	1	BENZOIC ACID, 4-(((6R)-7-CARBOXY-6-HYDROXYHEPTYL)THIO)-/CN
E9	1	BENZOIC ACID, 4-(((6R)-TETRAHYDRO-5-OXO-6-((4-(PHOSPHONOOXY)BENZOYL)AMINO)-1,4-THIAZEPIN-4(5H)-YL)METHYL)-, 1-METHYL ESTER/CN
E10	1	BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7

```
                    ,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
                    NDOL-2(1H)-YL)METHYL)-/CN
E11           1     BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7
                    ,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
                    NDOL-2(1H)-YL)METHYL)-, METHYL ESTER/CN
E12           1     BENZOIC ACID, 4-(((6S)-OCTAHYDRO-6-((4-HYDROXYPHENYL)METHYL)
                    -2-METHYL-4,7-DIOXO-1-(((PHENYLMETHYL)AMINO)CARBONYL)-8H-PYR
                    AZINO(2,1-C)(1,2,4)TRIAZIN-8-YL)METHYL)-/CN

=> e Benzoic acid, 4-(((6-oxo-6H-dibenzo(b,d)pyran-3-yl)oxy)methyl)-/cn
E1            1     BENZOIC ACID, 4-(((6-O-ACETYL-2,3,4-TRIS-O-(PHENYLMETHYL)-.A
                    LPHA.-D-MANNOPYRANOSYL)OXY)METHYL)-3-NITRO-, METHYL ESTER/CN
E2            1     BENZOIC ACID, 4-(((6-OXO-2,4-CYCLOHEXADIEN-1-YLIDENE)METHYL)
                    AMINO)-, METHYL ESTER/CN
E3            1 --> BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHY
                    L)-/CN
E4            1     BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHY
                    L)-, METHYL ESTER/CN
E5            1     BENZOIC ACID, 4-(((6-QUINOXALINYLAMINO)THIOXOMETHYL)AMINO)-,
                     METHYL ESTER/CN
E6            1     BENZOIC ACID, 4-(((6R)-6-(((2S)-2-(ACETYLAMINO)-1-OXO-3-(4-(
                    PHOSPHONOOXY)PHENYL)PROPYL)AMINO)TETRAHYDRO-5-OXO-1,4-THIAZE
                    PIN-4(5H)-YL)METHYL)-, 1-METHYL ESTER/CN
E7            1     BENZOIC ACID, 4-(((6R)-7-CARBOXY-6-HYDROXYHEPTYL)THIO)-/CN
E8            1     BENZOIC ACID, 4-(((6R)-TETRAHYDRO-5-OXO-6-((4-(PHOSPHONOOXY)
                    BENZOYL)AMINO)-1,4-THIAZEPIN-4(5H)-YL)METHYL)-, 1-METHYL EST
                    ER/CN
E9            1     BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7
                    ,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
                    NDOL-2(1H)-YL)METHYL)-/CN
E10           1     BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7
                    ,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
                    NDOL-2(1H)-YL)METHYL)-, METHYL ESTER/CN
E11           1     BENZOIC ACID, 4-(((6S)-OCTAHYDRO-6-((4-HYDROXYPHENYL)METHYL)
                    -2-METHYL-4,7-DIOXO-1-(((PHENYLMETHYL)AMINO)CARBONYL)-8H-PYR
                    AZINO(2,1-C)(1,2,4)TRIAZIN-8-YL)METHYL)-/CN
E12           1     BENZOIC ACID, 4-(((6S,9.ALPHA.,11.ALPHA.,13E,15S)-6,9-EPOXY-
                    11,15-DIHYDROXY-1-OXOPROSTA-7,13-DIEN-1-YL)AMINO)-/CN

=> e3
L18           1 "BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHYL)-
                "/CN

=> d l18

L18  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS
RN   314744-77-9  REGISTRY
CN   Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
     (9CI)  (CA INDEX NAME)
MF   C21 H14 O5
SR   Chemical Library
LC   STN Files:   CHEMCATS
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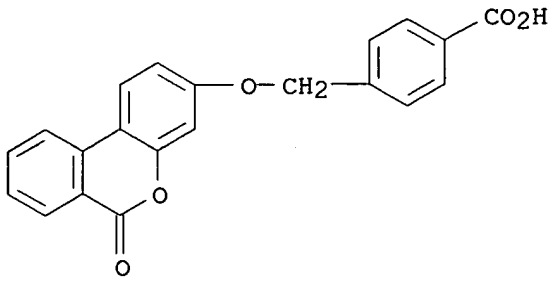


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> file chemcats
COST IN U.S. DOLLARS — SINCE FILE ENTRY: TOTAL SESSION

FULL ESTIMATED COST — 7.10 — 610.43

FILE 'CHEMCATS' ENTERED AT 09:13:31 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE LAST UPDATED 21 JUNE 2003 (20030621UP)

For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow prompt. For the list of suppliers currently in the file, enter HELP SPA, HELP SPBC, HELP SPDH, HELP SPIN, HELP SPOP, and HELP SPQZ. For the list of current catalogs, enter HELP CTA, HELP CTBC, HELP CTDH, HELP CTIN, HELP CTOP, and HELP CTQZ.

This database is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this database.

CHEMCATS now contains more than 5 million records. See HELP CONTENT and NEWS FILE for details.

=> l16
L19 22 L16

=> d l1911-22 ti
'L1911-22' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'
'TI' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'

The following are valid formats:

The default display format is IDE.

ALL ---- AN, CO, PD, ON, CN, RN, ST, Purity, Impurity, product identifiers, product notes, STR, product text (properties, regulatory information, references, prices, warnings, miscellaneous fields), CO, CA, CY, TX (products, terms, and conditions; products and services;

packaging and shipping; safety and handling; other supplier information)
COMP --- AN, CO, PD, CO, TX
IDE ---- AN, CO, PD, ON, CN, RN, LSF, ST, STR
MISC --- AN, miscellaneous product information fields
PINFO -- AN, pricing information text
PRICE -- AN, prices, quantities
PROD --- AN, product text
PROP --- AN, properties
REF ---- AN, references
REGS --- AN, regulatory information
SAFE --- AN, product warnings
SINFO -- AN, safety text
HIT ---- All fields containing hit terms
KWIC --- All hit terms plus 20 words on either side
OCC ---- List of display fields containing hit terms

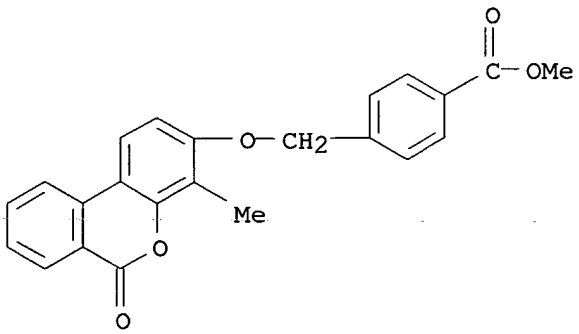
Hit terms will be highlighted in all displayable fields.

To display a particular field or fields, enter the display field codes. For a list of display field codes, enter 'HELP DFIELDS' at an arrow prompt (=>). Examples include: 'KWIC'; 'CN RN'; 'IDE CO'. You may specify the formats and fields in any order, and the information will be displayed in the same order as the format specification.

The same formats (except for HIT, KWIC, and OCC) may be used with the DISPLAY ACC command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (IDE):ide

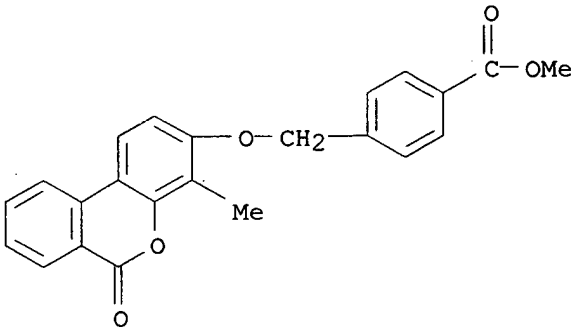
L19 ANSWER 1 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:2193953 CHEMCATS
Catalog Name (CO): ChemDiv, Inc. Product Library
Publication Date (PD): 25 Apr 2003
Order Number (ON): 3330-4466
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **307551-62-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



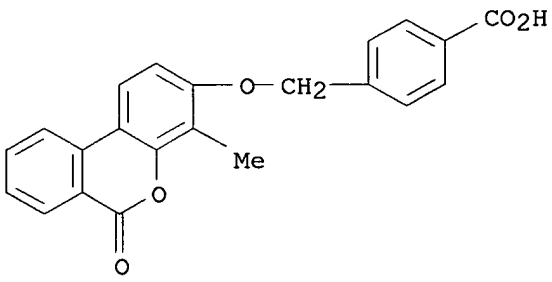
=> d l19 1-22 ide

L19 ANSWER 1 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2003:2193953 CHEMCATS
Catalog Name (CO): ChemDiv, Inc. Product Library
Publication Date (PD): 25 Apr 2003
Order Number (ON): 3330-4466
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **307551-62-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

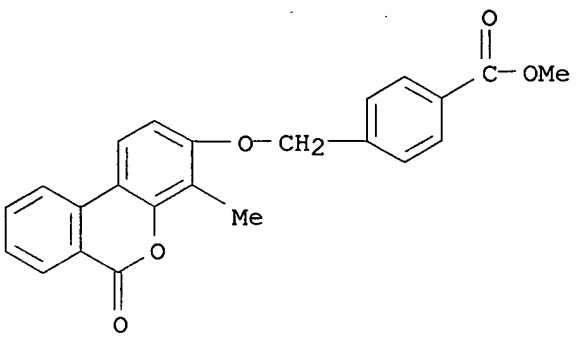


L19 ANSWER 2 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:884552 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7210430945
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
CAS Registry No. (RN): **314744-95-1**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

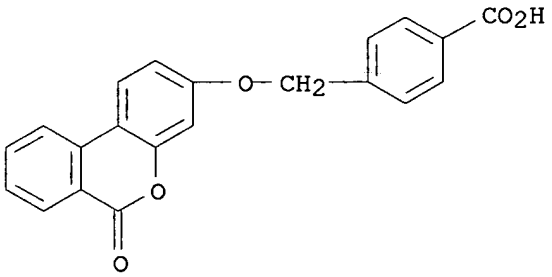


L19 ANSWER 3 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:884551 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7210430944
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
Synonym (CN): Also sold under Ambinter order number(s) F0398-0417, t0310-3431
CAS Registry No. (RN): **307551-62-8**

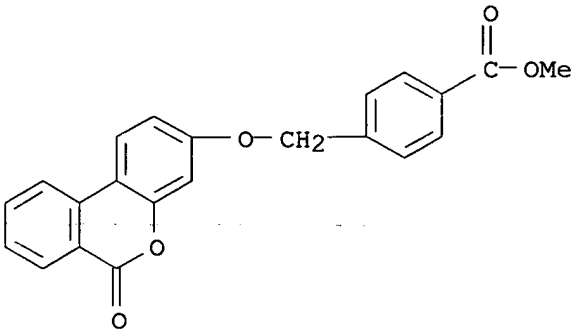
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



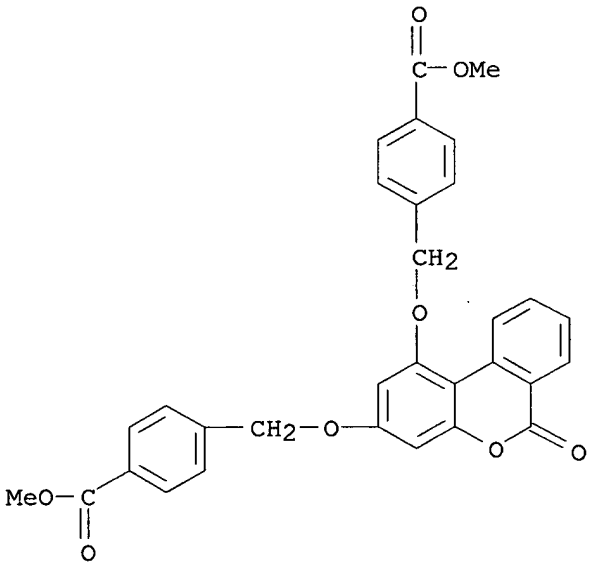
L19 ANSWER 4 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:884511 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7210430903
Chemical Name (CN): Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
CAS Registry No. (RN): **314744-77-9**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



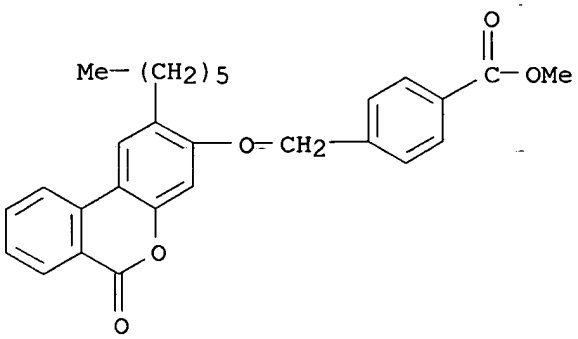
L19 ANSWER 5 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:884510 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7210430902
Chemical Name (CN): Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
Synonym (CN): Also sold under Ambinter order number(s) F0398-0388
CAS Registry No. (RN): **307551-40-2**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



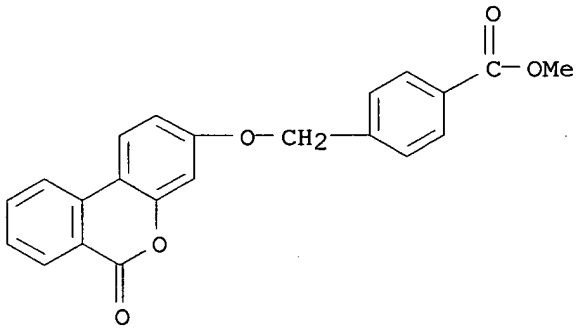
L19 ANSWER 6 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:2833186 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): t0304-3777
Chemical Name (CN): Benzoic acid, 4,4'-[(6-oxo-6H-dibenzo[b,d]pyran-1,3-diyl)bis(oxymethylene)]bis-, dimethyl ester
CAS Registry No. (RN): **438035-34-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



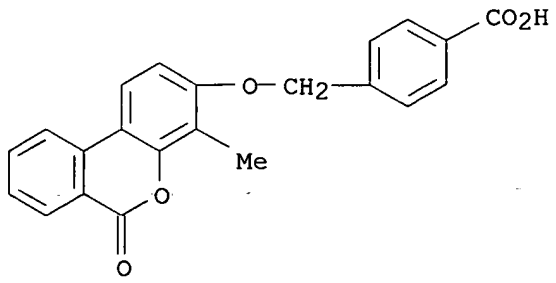
L19 ANSWER 7 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:2800180 CHEMCATS
Catalog Name (CO): Interchim Intermediates
Publication Date (PD): 9 Jul 2002
Order Number (ON): 7212010324
Chemical Name (CN): Benzoic acid, 4-[[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **405917-31-9**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



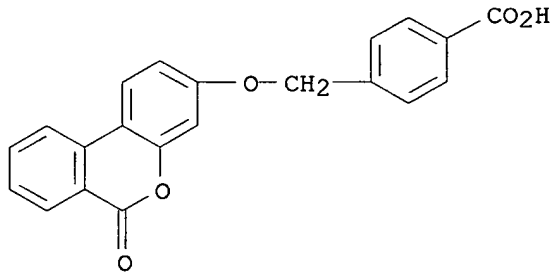
L19 ANSWER 8 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:2796908 CHEMCATS
Catalog Name (CO): Interchim Intermediates
Publication Date (PD): 9 Jul 2002
Order Number (ON): 7210430902
Chemical Name (CN): Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **307551-40-2**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



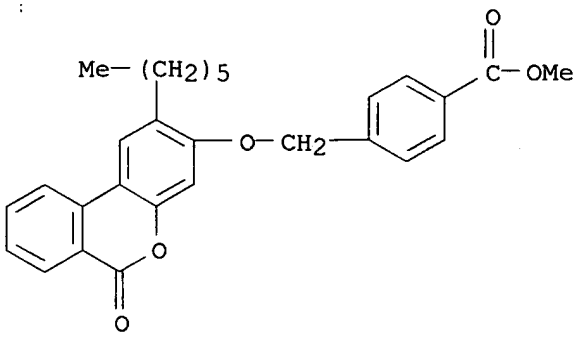
L19 ANSWER 9 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:2768171 CHEMCATS
Catalog Name (CO): Interchim Intermediates
Publication Date (PD): 9 Jul 2002
Order Number (ON): 7210430945
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
CAS Registry No. (RN): **314744-95-1**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



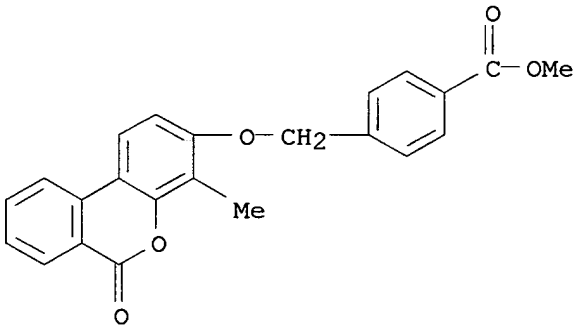
L19 ANSWER 10 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:2768153 CHEMCATS
Catalog Name (CO): Interchim Intermediates
Publication Date (PD): 9 Jul 2002
Order Number (ON): 7210430903
Chemical Name (CN): Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
CAS Registry No. (RN): **314744-77-9**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



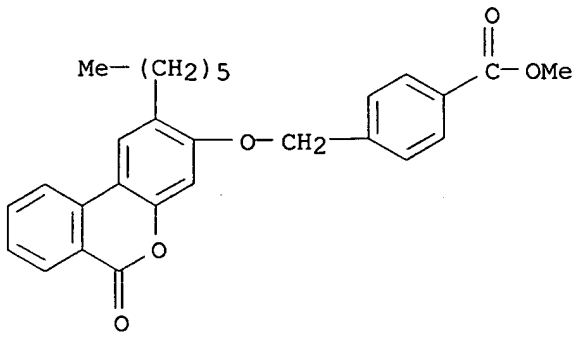
L19 ANSWER 11 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:2276618 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7212010324
Chemical Name (CN): Benzoic acid, 4-[[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **405917-31-9**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



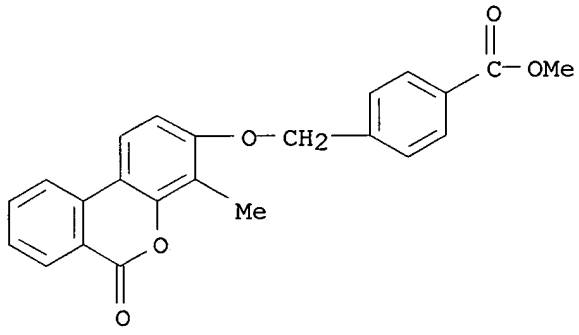
L19 ANSWER 12 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:2147072 CHEMCATS
Catalog Name (CO): Interchim Intermediates
Publication Date (PD): 9 Jul 2002
Order Number (ON): 3330-4466
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
Synonym (CN): Also sold under Interchim order number(s) 7210430944, F0398-0417
CAS Registry No. (RN): **307551-62-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



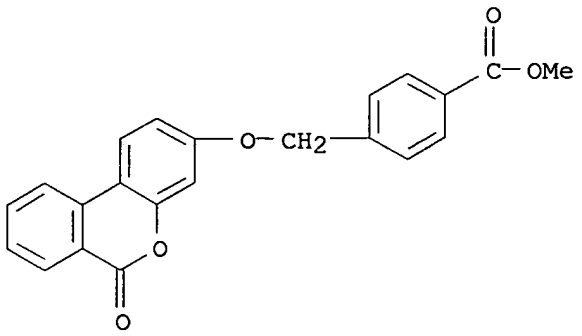
L19 ANSWER 13 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:1324350 CHEMCATS
Catalog Name (CO): Otava Stock Chemicals
Publication Date (PD): 28 May 2003
Order Number (ON): 7212010324
Chemical Name (CN): Benzoic acid, 4-[[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **405917-31-9**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



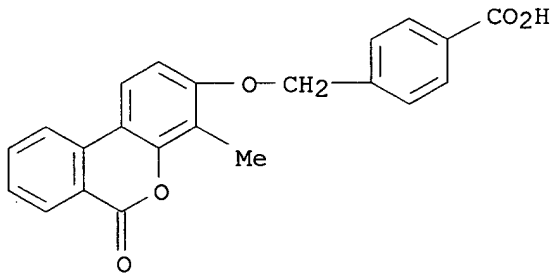
L19 ANSWER 14 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:607872 CHEMCATS
Catalog Name (CO): ChemBridge Product List
Publication Date (PD): 17 Jan 2002
Order Number (ON): 6166000
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **307551-62-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 15 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2002:605953 CHEMCATS
Catalog Name (CO): ChemBridge Product List
Publication Date (PD): 17 Jan 2002
Order Number (ON): 6145952
Chemical Name (CN): Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **307551-40-2**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 16 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2001:131979 CHEMCATS
Catalog Name (CO): Otava Chemical Collection
Publication Date (PD): 21 Apr 2003
Order Number (ON): 7210430945
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
CAS Registry No. (RN): **314744-95-1**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 17 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2001:131961 CHEMCATS
Catalog Name (CO): Otava Chemical Collection
Publication Date (PD): 21 Apr 2003
Order Number (ON): 7210430903
Chemical Name (CN): Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
CAS Registry No. (RN): **314744-77-9**
Supplementary Term (ST): CHEMICAL LIBRARY
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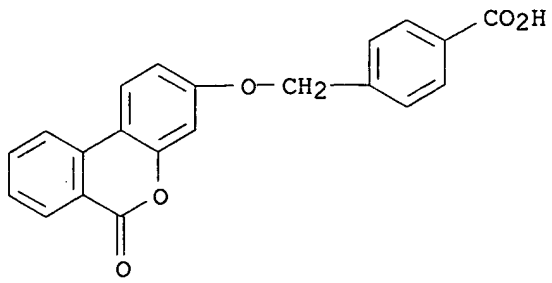
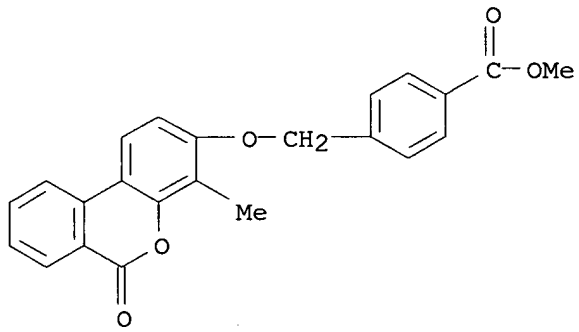
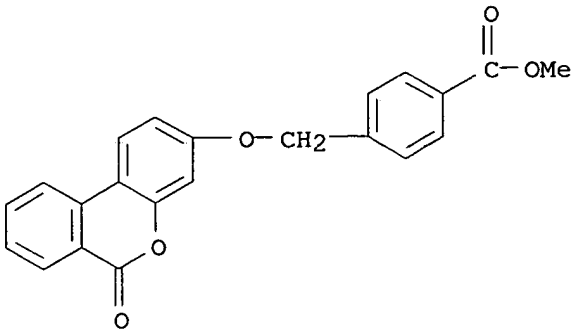


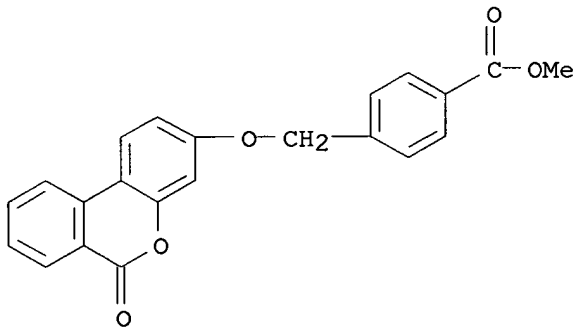
L19 ANSWER 18 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2000:1065757 CHEMCATS
Catalog Name (CO): Otava Stock Chemicals
Publication Date (PD): 28 May 2003
Order Number (ON): 7210430944
Chemical Name (CN): Benzoic acid, 4-[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **307551-62-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



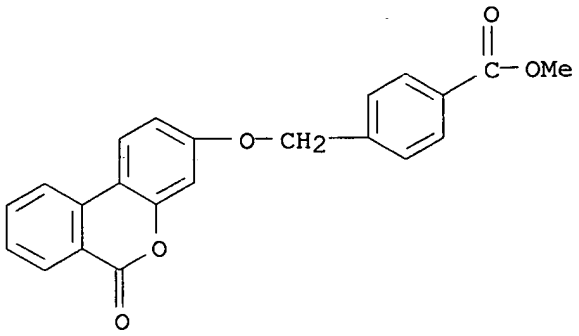
L19 ANSWER 19 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2000:1065735 CHEMCATS
Catalog Name (CO): Otava Stock Chemicals
Publication Date (PD): 28 May 2003
Order Number (ON): 7210430902
Chemical Name (CN): Benzoic acid, 4-[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): **307551-40-2**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



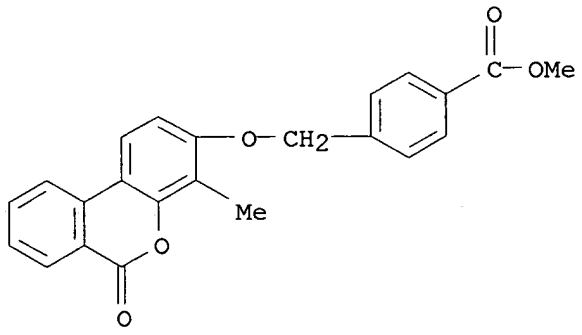
L19 ANSWER 20 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2000:899357 CHEMCATS
Catalog Name (CO): SALOR
Publication Date (PD): 15 Jan 2003
Order Number (ON): R632457
Chemical Name (CN): METHYL 4-(((6-OXO-6H-BENZO(C)CHROMEN-3-YL)OXY)METHYL)BENZOATE
CAS Registry No. (RN): **307551-40-2**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 21 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2000:897302 CHEMCATS
Catalog Name (CO): SALOR
Publication Date (PD): 15 Jan 2003
Order Number (ON): R609854
Chemical Name (CN): METHYL 4-(((6-OXO-6H-BENZO(C)CHROMEN-3-YL)OXY)METHYL)BENZOATE
CAS Registry No. (RN): **307551-40-2**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 22 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2000:434091 CHEMCATS
Catalog Name (CO): SALOR
Publication Date (PD): 15 Jan 2003
Order Number (ON): R503738
Chemical Name (CN): 4-(4-METHYL-6-OXO-6H-BENZO(C)CHROMEN-3-YLOXYMETHYL)-BENZOIC ACID METHYL ESTER
CAS Registry No. (RN): **307551-62-8**
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



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NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
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NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
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NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN
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NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 20	EVENTLINE will be removed from STN
NEWS 28	Mar 24	PATDPAFULL now available on STN
NEWS 29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 30	Apr 11	Display formats in DGENE enhanced
NEWS 31	Apr 14	MEDLINE Reload
NEWS 32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 33	Jun 13	Indexing from 1947 to 1956 added to records in CA/CAPLUS
NEWS 34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 35	Apr 28	RDISCLOSURE now available on STN
NEWS 36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS 38	May 15	Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39	May 16	CHEMREACT will be removed from STN
NEWS 40	May 19	Simultaneous left and right truncation added to WSCA
NEWS 41	May 19	RAPRA enhanced with new search field, simultaneous left and right truncation
NEWS 42	Jun 06	Simultaneous left and right truncation added to CBNB
NEWS 43	Jun 06	PASCAL enhanced with additional data
NEWS 44	Jun 20	2003 edition of the FSTA Thesaurus is now available
NEWS 45	Jun 25	HSDB has been reloaded

NEWS EXPRESS	April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
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NEWS INTER	General Internet Information

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NEWS PHONE     Direct Dial and Telecommunication Network Access to STN
NEWS WWW       CAS World Wide Web Site (general information)

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FILE COVERS 1907 - 7 Jul 2003  VOL 139 ISS 2
FILE LAST UPDATED: 6 Jul 2003  (20030706/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> arotinoids
L1          54 AROTINOIDS

=> retinobenzoic
L2          40 RETINOBENZOIC

=> l1 and l2
L3           0 L1 AND L2

=> phenan?
L4       62851 PHENAN?

=> l1 and l4
L5           0 L1 AND L4

=> d l1 44-54 ti

L1   ANSWER 44 OF 54  CAPLUS  COPYRIGHT 2003 ACS
```

TI The effects of **arotinoids** on rat mammary carcinogenesis

L1 ANSWER 45 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Retinoid-induced changes of lipid synthesis in cultured human epidermal keratinocytes

L1 ANSWER 46 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Diazacholesterol-induced ichthyosis in the hairless mouse

L1 ANSWER 47 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Sulfur-containing **arotinoids**, a new class of retinoids

L1 ANSWER 48 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Synergistic effect of retinoic acid on DNA synthesis by prostaglandin F2.alpha. stimulated Swiss 3T3 cells

L1 ANSWER 49 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Effects of **arotinoids** upon murine embryonal carcinoma cells

L1 ANSWER 50 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Retinoic acid enhances the initiation of DNA synthesis stimulated by prostaglandin F2.alpha. in Swiss 3T3 cells

L1 ANSWER 51 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Affinity therapeutics. 1. Selective incorporation of 2-thiouracil derivatives in murine melanomas. Cytostatic activity of 2-thiouracil **arotinoids**, 2-thiouracil retinoids, **arotinoids**, and retinoids

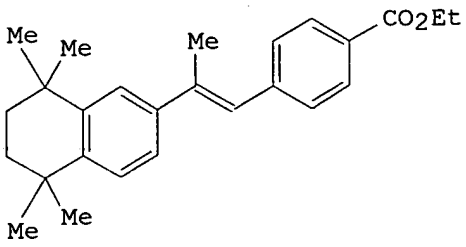
L1 ANSWER 52 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology

L1 ANSWER 53 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Structure-activity relationship of retinoids in fetal rat bone cultures

L1 ANSWER 54 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI **Arotinoids**, a new class of highly active retinoids

=> d l1 52-54 ti fbib abs

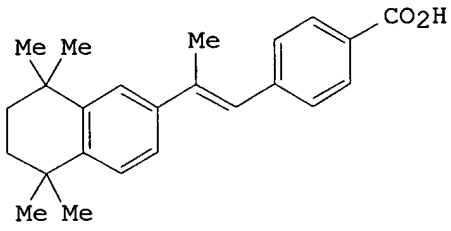
L1 ANSWER 52 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology
AN 1982:141529 CAPLUS
DN 96:141529
TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology
AU Bollag, Werner
CS Pharma Res. Dep., F. Hoffmann-La Roche und Co. Ltd., Basel, Switz.
SO Cancer Chemotherapy and Pharmacology (1981), 7(1), 27-9
CODEN: CCPHDZ; ISSN: 0344-5704
DT Journal
LA English
GI



I

AB **Arotinoids** are a new class of retinoids with particular biol. properties. Arotinoid Ro 13-6298 (I) [71441-09-3] in minute quantities leads to regression of chem. induced papillomas of the skin of mice. The ratio between the antipapilloma effect and the toxic syndrome of hypervitaminosis A is very favorable. Ro 13-6298 also has a therapeutic influence on chem. induced skin carcinomas in mice. As the papilloma model has proved to be suitable for screening for antipsoriatic and antikeratinizing properties as well as for antineoplastic screening, artinoids might be useful in human clin. dermatol. and oncol.

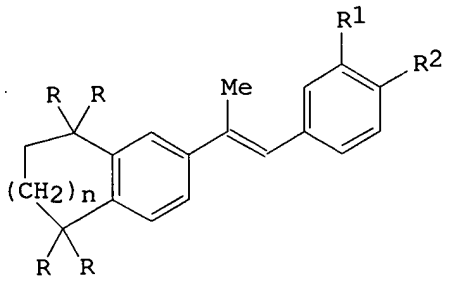
L1 ANSWER 53 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI Structure-activity relationship of retinoids in fetal rat bone cultures
AN 1981:525879 CAPLUS
DN 95:125879
TI Structure-activity relationship of retinoids in fetal rat bone cultures
AU Kistler, Andreas
CS Biol. Pharm. Res. Dep., F. Hoffmann-La Roche Co. Ltd., Basel, CH-4002, Switz.
SO Calcified Tissue International (1981), 33(3), 249-54
CODEN: CTINDZ; ISSN: 0171-967X
DT Journal
LA English
GI



I

AB The structure-activity relation of 29 retinoids was investigated in fetal rat bone organ cultures. Retinoids induced the release of proteoglycan followed by cartilage tissue breakdown. The loss of RNA was used as a parameter for cartilage resorption. During 6 days of incubation, RNA decreased up to 80% in the presence of active retinoids. The ED40 was detd. from dose-response curves of the various retinoids. The new compds., called **arotinoids**, which contained the retinoic acid C skeleton in a fixed cisoid geometric conformation, were up to 200 times more active than all-trans-.beta.-retinoic acid. The most active compd. was I [71441-28-6]. Several lines of evidence indicated that the carboxylic acid end group was essential for the activity of retinoids in fetal bone cultures. These new, highly active retinoids might be an excellent tool to investigate whether the retinoid action is mediated by specific cellular retinoid binding proteins.

L1 ANSWER 54 OF 54 CAPLUS COPYRIGHT 2003 ACS
TI **Arotinoids**, a new class of highly active retinoids
AN 1980:586020 CAPLUS
DN 93:186020
TI **Arotinoids**, a new class of highly active retinoids
AU Loeliger, Peter; Bollag, Werner; Mayer, Hans
CS F. Hoffmann-La Roche and Co. Ltd., Basel, CH 4002, Switz.
SO European Journal of Medicinal Chemistry (1980), 15(1), 9-15
CODEN: EJMCA5; ISSN: 0009-4374
DT Journal
LA English
GI



I

AB A new class of retinoids, named **arotinoids** (I), R = H or Me, R1 = H, R2 = COEt, n = 0; R = R1 = Me, R2 = CO2Et, n = 1; R = Me, R1 = H, R2 = H, Me, CHO, CH2OH, CH2OMe, CH2OAc, CO2H, CO2Et, CO2CHMe2, CO2CMe3 or CONHEt, n = 1), which had up to 10 times more favorable therapeutic ratio for papilloma regression than retinoic acid (II) were prepd. by the Wittig reaction of (1-arylethyl)triphenylphosphonium bromides with benzaldehydes. E.g., Me 5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthyl ketone was reduced, the alc. converted to the bromide, and this was quaternized with Ph3P and reacted with 4-HCOC6H4CO2Et to give (E)-I (R = Me, R1 = H, R2 = CO2Et, n = 1), which had therapeutic potency in the antipapilloma test 8000 times that of II while the toxic hypervitaminosis A effects were increased by 800 times.

```
=> tricyc?
L6       30539 TRICYC?

=> d his

     (FILE 'HOME' ENTERED AT 13:10:23 ON 07 JUL 2003)

     FILE 'CAPLUS' ENTERED AT 13:10:30 ON 07 JUL 2003
L1           54 AROTINOIDS
L2           40 RETINOBENZOIC
L3            0 L1 AND L2
L4        62851 PHENAN?
L5            0 L1 AND L4
L6        30539 TRICYC?

=> l1 and l6
L7            0 L1 AND L6

=> ?arotinoids
L8          298 ?AROTINOIDS

=> carotinoids
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L9 209 CAROTINOIDS

=> l8 not l9
L10 89 L8 NOT L9

=> l10 not l1
L11 35 L10 NOT L1

=> benzo?
L12 475881 BENZO?

=> l11 and l12
L13 15 L11 AND L12

=> d l13 1-15 ti

L13 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties

L13 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions

L13 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-**benzo**[b]thien-5-yl)-1-propenyl]**benzoate**, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-**benzofuranyl**)-1-propenyl] **benzoate**, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-3-hydroxy-1-propenyl]**benzoate** as potential metabolites of selected **heteroarotinoids** with fused five-membered rings

L13 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic cultures of ovarian carcinoma

L13 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]

L13 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic** acid-11-[14C]

L13 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**

L13 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI synthesis, receptor specificity and TGase activity of **heteroarotinoids**-anticancer agents

L13 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

L13 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**: crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] **benzoate**

L13 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Novel **heteroarotinoids**: synthesis and biological activity

L13 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**: analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples

L13 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Heteroarotinoid compounds as anticancer agents

L13 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**. Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells

L13 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]**benzoate**

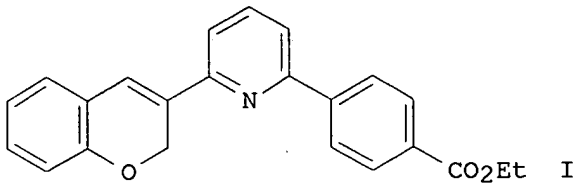
=> benzoarotinoid?
L14 0 BENZOAROTINOID?

=> d l13 1-15 ti fbib abs

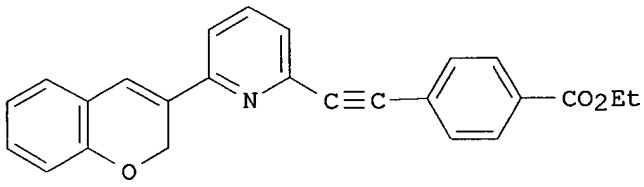
L13 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties
AN 2003:322782 CAPLUS
TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties
AU Weerasekare, G. Mahika; Berlin, K. Darrell; Sunkara, Haribabu; Ford, Warren T.
CS Oklahoma State University, Stillwater, OK, USA
SO Phosphorus, Sulfur and Silicon and the Related Elements (2003), 178(5), 993-1006
CODEN: PSSLEC; ISSN: 1042-6507
PB Taylor & Francis Ltd.
DT Journal
LA English
AB Synthetic methods were developed to prep. Et (E)-4-[2-(3,4-dihydro-2-n-octyl-1-oxy-2H-1-**benzothio**-pyran-6-yl)-1-propenyl] **benzoate** (1) and Et (E)-4-[2-(3,4-dihydro-2-n-octyl-2H-1-**benzothiopyran**-6-yl)-1-propenyl]**benzoate** (10). These are the first examples of **heteroarotinoids** which possess properties of liq. crystals. The properties were evaluated using differential scanning calorimetry and by use of polarizing microg. Both displayed textures which are typical of a smectic or cholesteric phase.

L13 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions
AN 2001:867362 CAPLUS
DN 136:151322
TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions
AU Alami, Mouad; Peyrat, Jean-Francois; Belachmi, Larbi; Brion, Jean-Daniel
CS Laboratoire de Chimie Therapeutique, associe au CNRS (BioCIS), Universite

Paris-Sud, Faculte de Pharmacie, Chatenay-Malabry, 92296, Fr.
SO European Journal of Organic Chemistry (2001), (22), 4207-4212
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 136:151322
GI



I

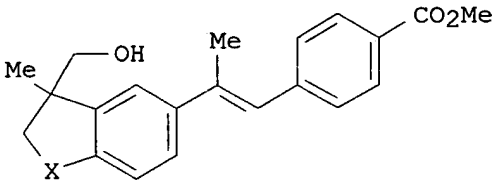


II

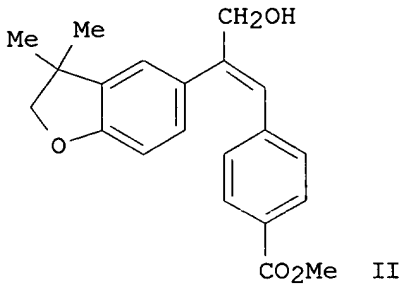
AB A convergent synthesis of **heteroarotinoids** bearing chromene rings in assocn. with pyridyl or ethynylpyridyl moieties, from 6-bromo-2-pyridylzinc chloride is described. This new functional heteroarylzinc reagent, readily accessible from 2,6-dibromopyridine, may undergo a selective palladium-catalyzed carbon-carbon bond-forming reaction to yield the corresponding 6-substituted-2-bromopyridines. Further manipulation of the remaining bromine atom to give the zinc deriv., and subsequent coupling with Et 4-iodobenzoate under palladium catalysis conditions afforded heteroarotinoid I. Coupling of the 6-substituted-2-bromopyridines or Me nicotinate triflate with appropriate alkynes under Sonogashira conditions give the corresponding **heteroarotinoids**, e.g. II.
RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-**benzo**[b]thien-5-yl)-1-propenyl]**benzoate**, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-**benzofuranyl**)-1-propenyl] **benzoate**, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-3-hydroxy-1-propenyl]**benzoate** as potential metabolites of selected **heteroarotinoids** with fused five-membered rings
AN 2001:691383 CAPLUS
DN 136:5846
TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-**benzo**[b]thien-5-yl)-1-propenyl]**benzoate**, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-**benzofuranyl**)-1-propenyl] **benzoate**, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-3-hydroxy-1-propenyl]**benzoate** as potential metabolites of selected **heteroarotinoids** with fused five-membered rings
AU Gale, Jonathan B.; Klucik, Jozef; Subramanian, Shankar; Berlin, K. Darrell
CS Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078,

USA
SO Organic Preparations and Procedures International (2001), 33(5), 487-499
CODEN: OPPIAK; ISSN: 0030-4948
PB Organic Preparations and Procedures, Inc.
DT Journal
LA English
OS CASREACT 136:5846
GI



I



II

AB The title compds. I (X = S), I (X= O), and II were prepd. were prepd. stareing from 2-aminothiophenol and 2-nitrophenol.
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic cultures of ovarian carcinoma
AN 2001:308164 CAPLUS
DN 135:251521
TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic cultures of ovarian carcinoma
AU Guruswamy, Suresh; Lightfoot, Stan; Gold, Michael A.; Hassan, Raffit; Berlin, K. Darrell; Ivey, R. Todd; Benbrook, Doris M.
CS Departments of Obstetrics and Gynecology and Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center, Oklahoma City, OK, 73190, USA
SO Journal of the National Cancer Institute (2001), 93(7), 516-525
CODEN: JNCIEQ; ISSN: 0027-8874
PB Oxford University Press
DT Journal
LA English
AB Background: Retinoic acid analogs, called retinoids, have shown promise in clin. trials in preventing breast and ovarian cancers. Classic retinoids bind to retinoic acid receptors, which regulate cell growth. Some novel retinoids, such as fenretinide, i.e., N-(4-hydroxyphenyl)retinamide (4-HPR), induce apoptosis through retinoic acid receptor-independent mechanisms; however, they appear to do so only at concns. above those achieved in clin. chemoprevention trials. At lower concns. (.ltoreq.1 .mu.M), 4-HPR acts like classic retinoids, by inducing differentiation

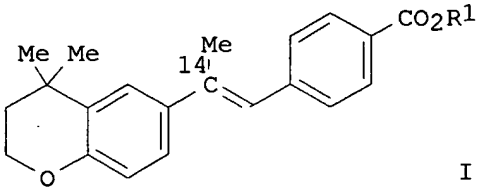
through a receptor-dependent mechanism. Our goal was to compare the effects of novel receptor-independent (apoptotic) retinoids with those of classic growth-inhibitory retinoids at clin. achievable doses on growth, differentiation, and apoptosis in ovarian tissue. Methods: Four receptor-independent (apoptotic) and seven growth-inhibitory retinoids, including synthetic, low-toxicity compds. called **heteroarotinoids**, were administered at concns. of 1 .mu.M to organotypic cultures of ovarian primary and cancer cell lines: OVCAR-3, Caov-3, and SK-OV-3. After fixation, embedding, and sectioning, the growth fraction was quantified by measuring expression of the proliferation marker Ki-67/myb, differentiation was assessed by expression of mucin, and apoptosis was evaluated by the TUNEL assay. Spearman correlation anal. was performed on the data, and all P values were two-sided. Results: All 11 retinoids reversed characteristics assocd. with the cancerous phenotype in all neoplastic cultures. Glandular structures were obsd. consistently in retinoid-treated, but not in untreated, OVCAR-3 and Caov-3 cultures. All retinoids decreased growth fractions, and some increased mucin expression. All receptor-independent retinoids and two receptor-dependent retinoids induced apoptosis, and the induction correlated significantly with increased expression of the mucin MUC1 ($r = .83$; $P = .03$). Retinoids with ester-linking groups did not induce apoptosis but decreased the growth fraction in correlation with MUC1 induction ($r = -.93$; $P = .02$). Conclusions: At clin. achievable concns., all retinoids tested decrease the growth fraction, induce differentiation and apoptosis. Induction of MUC1 expression is implicated in the mechanisms of action.

RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

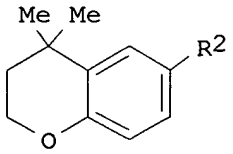
L13 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]
AN 1999:803609 CAPLUS
DN 132:293893
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]
AU Dhar, Arindam; Liu, Shengquan; Klucik, Jozef; Berlin, K. Darrell; Madler, Matora M.; Lu, Shennan; Ivey, R. Todd; Zacheis, David; Brown, Chad W.; Nelson, E. C.; Birckbichler, Paul J.; Benbrook, Doris M.
CS Departments Obstetrics Gynecology of Biochem., Molecular Biol. of Otorhinolaryngology and Urology, Univ. Oklahoma Health Sciences Center, Oklahoma City, OK, 73190, USA
SO Journal of Medicinal Chemistry (2000), 43(2), 303
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB On page 3606, under Discussion, lines 24 and 25, the ref. to Table 2 is incorrect; Table 1 is the correct ref. The cor. sentence is as follows: "The EC50 value of 6 nM and the 103% efficacy of 2 (Table 1), in comparison to that of 9-c-RA, indicate that 2 may be useful as a pharmaceutical agent for disorders of the skin.".

L13 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic** acid-11-[14C]
AN 1999:525825 CAPLUS
DN 131:310738
TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic** acid-11-[14C]
AU Liu, Shengquan; Berlin, K. Darrell; Simms-Kelley, Melissa D.; Nelson, Eldon C.; Benbrook, Doris M.

CS Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078, USA
SO Journal of Labelled Compounds & Radiopharmaceuticals (1999), 42(8), 789-796
CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
GI



I

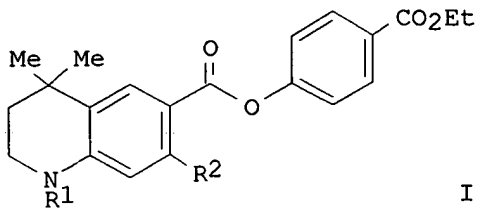


II

AB **Heteroarotinoids** may be useful in the treatment of skin disorders and a wide variety of cancers. A synthesis of the C-14 labeled heteroarotinoid, (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic** acid-11-[14C] (I; R1 = H) is described via a multistep procedure similar to that used to obtain the unlabeled compd. The latter has shown good activity in several assays compared to the std. trans-retinoic acid. Redn. of the carbonyl group in 4,4-dimethylchroman-6-yl Me ketone-(carbonyl-14C) (II; R2 = 13COMe) with LiAlH4 gave alc. II (R2 = 13CHMeOH). Phosphorylation with triphenyl-phospine hydrobromide in methanol led to the corresponding phosphonium salt II (R2 = 13CHMeP+Ph3Br-). Addn. of n-butyllithium to II (R2 = 13CHMeP+Ph3Br-) in ether at -78.degree.C generated the Wittig reagent in situ and to this was added Et 4-formylbenzoate. Workup and chromatog. afforded E-ester I (R1 = Me) and the Z-ester which were both hydrolyzed to labeled I. Labeled I was identical to the unlabeled isotopomer in terms of spectral data and m.p. The specific activity of I was detd. to be 57.2 .mu.Ci/mg.
RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**
AN 1999:521109 CAPLUS
DN 131:310737
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**
AU Dhar, Arindam; Liu, Shengquan; Klucik, Jozef; Berlin, K. Darrell; Madler, Matora M.; Lu, Shennan; Ivey, R. Todd; Zacheis, David; Brown, Chad W.; Nelson, E. C.; Birckbichler, Paul J.; Benbrook, Doris M.
CS Departments of Obstetrics Gynecology of Biochemistry Molecular Biology of Otorhinolaryngology and of Urology, University of Oklahoma Health Sciences

Center, Oklahoma City, OK, 73190, USA
SO Journal of Medicinal Chemistry (1999), 42(18), 3602-3614
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



I

AB Three **heteroarotinoids** contg. a nitrogen atom in the first ring and a C-O linking group between the two aryl rings were synthesized and evaluated for RAR and RXR retinoid receptor transactivation, tumor cell growth inhibition, and transglutaminase (TGase) induction. Et 4-(N,4,4-trimethyl-1,2,3,4-tetrahydroquinolinyl)**benzoate** (I; R1 = Me, R2 = H) contained an N-CH3 group and activated all retinoid receptors except for RAR.gamma.. Increasing the hydrophobicity around the rings with analogs Et 4-(N,4,4,7-tetramethyl-1,2,3,4-tetrahydroquinolin-6-oyloxy)**benzoate** (I; R1 = R2 = Me) and Et 4-(4,4-dimethyl-N-isopropyl-1,2,3,4-tetrahydroquinolin-6-oyloxy)**benzoate** (I; R1 = CHMe2, R2 = H) increased the potency and specificity for RAR.alpha., RAR.beta., and RXR.alpha., compared to I (R1 = Me, R2 = H), but had little effect on RXR.beta. and RXR.gamma. activation. Although I (R1 = Me, CHMe2, R2 = H) were unable to activate RAR.gamma., I (R1 = R2 = Me) did activate this receptor with efficacy and high potency equal to that of 9-cis-retinoic acid (II). All three **heteroarotinoids** exhibited 5-8-fold greater specificities for RAR.beta. over RAR.alpha.. In addn., esters I inhibited the growth of two cell lines each derived from cervix, vulvar, ovarian, and head/neck tumors with similar efficiencies to that of IIthrough a mechanism independent of apoptosis. The vulvar cell lines were the most sensitive, and the ovarian lines were the least sensitive. Ester was similar to I (R1 = Me, CHMe2; R2 = H) except that I (R1 = R2 = Me) was a much more potent growth inhibitor of the two vulvar cell lines, which is consistent with strong RAR.gamma. activation by I (R1 = R2 = Me) [but not by I (R1 = Me, CHMe2; R2 = H)] and the high levels of RAR.gamma. expression in skin. All three **heteroarotinoids** induced prodn. of TGase, a marker of retinoid activity in human erythroleukemic cells. Esters I (R1 = R2 = Me; R1 = CHMe2, R2 = H) were the more potent TGase activators than I (R1 = Me R2 = H) , in agreement with the stronger activation of the RAR receptors by I (R1 = R2 = Me; R1 = CHMe2, R2 = H). The biol. activities of these agents, and the RAR.gamma. potency of I (R1 = R2 = Me) in particular, demonstrate the promise of these compds. as pharmaceutics for cancer and skin disorders.

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI synthesis, receptor specificity and TGase activity of **heteroarotinoids**-anticancer agents
AN 1998:147324 CAPLUS
DN 128:204998
TI synthesis, receptor specificity and TGase activity of **heteroarotinoids**-anticancer agents
IN Berlin, Kenneth Darrel; Subramanian, Shanker; Nelson, Eldon Carl; Madler,

Matora May; Patterson, Manford Kenneth, Jr.; Birckbichler, Paul Joseph; Benbrook, Doris Mangiaracina

PA Board of Regents for Oklahoma State University, USA

SO PCT Int. Appl., 93 pp.
CODEN: PIXXD2

DT Patent

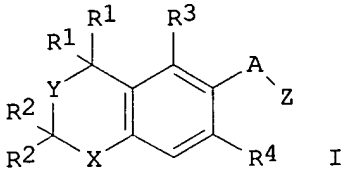
LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9807716	A2	19980226	WO 1997-US14720	19970821
W: AU, CA, CN, JP				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
			US 1996-24521P P	19960823
AU 9740805	A1	19980306	AU 1997-40805	19970821
			US 1996-24521P P	19960823
			WO 1997-US14720W	19970821

OS MARPAT 128:204998

GI



I

AB Synthesis of heteroarotinoid structures (I) [R1 = H, Me; R2 = H, Me; R3 = H, Me; R4 = H, Me, OMe; A = CO2, O2C, CONH, CONOH, CONOMe, NHCO, C(Me)=CH, COCH=CH; X = O, S, SO, SO2, NMe, NEt, NPr, NCHMe2, CMe2; Y = CH2, O, S; Z = C6H4-4-CO2R, C6H4-3-CO2R, C6H3-3-Me-4-CO2R, C6H3-2-Me-4-CO2R , CH=CHCH=CHCO2R, CH=CHC(Me)=CHCO2R; R = H, Me, Et, Pr, CHMe2] partially related to trans-retinoic acid through the basic, fused-ring framework and having receptor specificity as well as activity in stimulating formation of the enzyme transglutaminase as a marker for anticancer activity is reported. Thus, I (R1=R2 = Me, R3=R4 = H, Y = CH2, X = S, A = NHCO, Z = C6H3-2-Me-4-CO2R, R = H) (II) is prepd. in 68% yield by NaOH hydrolysis of the corresponding ester in ethanol formed by the condensation of 6-amino-2,3-dihydro-2,2,4,4-tetramethyl-2H-1-**benzothiopyran** with monomethyl terephthaloyl chloride. II shows an R value of 0.76 as compared to trans-retinoic acid in TGase assay.

L13 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

AN 1997:638457 CAPLUS

DN 127:307506

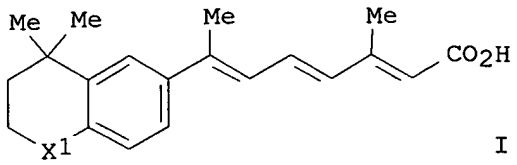
TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

AU Benbrook, Doris M.; Madler, Matora M.; Spruce, Lyle W.; Birckbichler, Paul J.; Nelson, Eldon C.; Subramanian, Shankar; Weerasekare, G. Mahika; Gale, Jonathan B.; Patterson, Manford K., Jr.; Wang, Binghe; Wang, Wei; Lu, Shennan; Rowland, Tami C.; DiSivestro, Paul; Lindamood, Charles; Hill, Donald L.; Berlin, K. Darrell

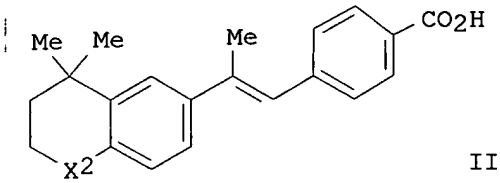
CS Departments of Obstetrics Gynecology Urology and Medicinal Chemistry and Pharmaceutics, University of Oklahoma Health Sciences Center, Oklahoma City, OK, 73L90, USA

SO Journal of Medicinal Chemistry (1997), 40(22), 3567-3583

CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



I

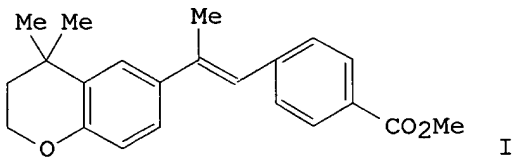


II

AB A series of retinoids, contg. heteroatoms in a cyclic ring and called **heteroarotinoids**, were synthesized, and their biol. activity was evaluated using tissue culture lines that have measurable responses to trans-retinoic acid (t-RA). Transglutaminase (TGase) was assessed in the human erythroleukemia cell line (GMO6141A) as an indicator of differentiation and apoptosis. Proliferation was evaluated in a human cervical cell line, CC-1, which exhibits dose-dependent alterations in growth rate in response to treatment with trans-retinoic acid. Activation of nuclear retinoic acid receptors was detd. in a reporter cell line established from CC-1. The reporter line, called CC-B, contains a reporter gene controlled by a retinoic acid responsive element (RARE) and a thymidine kinase (tk) promoter. Treatment of the CC-B line with the **heteroarotinoids** resulted in a dose-responsive and retinoid-dependent regulation of reporter gene expression. The **heteroarotinoids** exhibited activity in all assays and correlated in a statistically significant manner between assays. RARE transactivation activity in CC-B cells correlated with induction of TGase in GMO6141A (R = 0.96) and with a decrease in the growth rate of CC-1 cells (R = -0.90). The ability of the selected **heteroarotinoids** to induce differentation, inhibit proliferation, and activate nuclear receptors demonstrates the chemotherapeutic potential of these agents. In view of the biol. activity cited, an in vivo toxicity study was conducted on male B6D2F1 mice with three **heteroarotinoids**, namely (2E,4E,6E)-3,7-dimethyl-7-(1,2,3,4-tetrahydro-4,4-dimethylthiochroman-6-yl)-2,4,6-heptatrienoic acid (I; X1 = S), (2E,4E,6E)-3,7-dimethyl-7-(1,2,3,4-tetrahydro-4,4-dimethylchroman-6-yl)-2,4,6-heptatrienoic acid (I; X1 = O), and (E)-p-[2-(4,4-dimethylchroman-6-yl)propenyl]**benzoic** acid (II; X2 = O). The mice were used with gavage of **heteroarotinoids** in corn oil [0.1, 0.2, 0.4, or 0.8 mg/kg] and with 0.01 or 0.05 mg/kg of (E)-4-[2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-1-propenyl]**benzoic** acid [TTNPB (II; X2 = CMe2)] as ref. controls. The target organs affected in the mice by the three **heteroarotinoids** were those typically assocd. with trans-retinoic acid (III) toxicity. The max. tolerated dose (MTD) of 13 was 9.4 mg/kg/day, which was equal in toxicity to that of III and 1000-fold less toxic than TTNPB. The MTDs of I were 34 and 32 mg/kg/day,

resp., which is 3-fold less toxic than III and 3000-fold less toxic than TTNPB. The 3000-fold reduced toxicity, compared with only a 27% redn. biol. activity of I with respect to that of TTNPB, obsd. in our assays indicates a good therapeutic ratio of these **heteroarotinoids** over the parent compd. The biol. activity and reduced toxicity of these **heteroarotinoids** demonstrate the potential efficacy as anticancer agents.

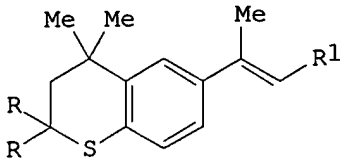
L13 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**: crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] **benzoate**
AN 1992:6745 CAPLUS
DN 116:6745
TI **Heteroarotinoids**: crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] **benzoate**
AU Welsh, William J.; Cody, Vivian; Suwinskat, Kinga; Berlin, K. Darrell; Rajadhyaksha, Shirish N.; Subramanian, Shankar; Verma, A. K.
CS Dep. Chem., Univ. Missouri, St. Louis, MO, 63121, USA
SO Structural Chemistry (1991), 2(5), 515-22
CODEN: STCHES; ISSN: 1040-0400
DT Journal
LA English
GI



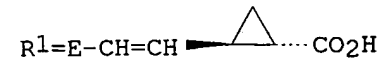
I

AB Crystal structures and MM2P mol. mechanics force-field and AM1 MO calcns. were performed on Me (E)- and Me (Z)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl]**benzoate** (I) and confirmed that the calcd. mol. structures are in good agreement with the obsd. crystallog. conformations which show that both isomers have a twist-sofa oxo ring conformation and nearly perpendicular arom. ring systems, resp. Full relaxation MM2P conformational energy profiles for the rotation about the propenyl bridge indicate that the max. energy barrier is less than 3.5 kcal/mol.

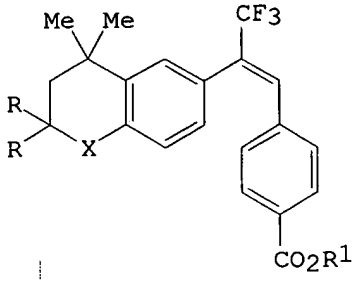
L13 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Novel **heteroarotinoids**: synthesis and biological activity
AN 1991:114595 CAPLUS
DN 114:114595
TI Novel **heteroarotinoids**: synthesis and biological activity
AU Spruce, Lyle W.; Gale, Jonathan B.; Berlin, K. Darrell; Verma, A. K.; Breitman, Theodore R.; Ji, Xinhua; Van der Helm, Dick
CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
SO Journal of Medicinal Chemistry (1991), 34(1), 430-9
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 114:114595
GI



I, R=Me, $R^1=C_6H_4CO_2Me$-4
II, R=Me, $R^1=C_6H_4CO_2H$-4
IV, R=H, R^1=E,E-CH=CHCMe=CO_2H
V, R=Me, R^1=E,Z-CH=CHCMe=CO_2H



VI, R=H, R^1=E-CH=CH



VII, R=R^1=Me, X=S
VIII, R=Me, R^1=H, X=S
IX, R=H, R^1=Me, X=S
X, R=R^1=H, X=S
XI, R=H, R^1=Me, X=O
XII, R=R^1=H, X=O

AB Thirteen **heteroarotinoids** were synthesized. The key step in each prepn. was the condensation of the appropriate chroman-, thiochroman-, or **benzothienyl**-substituted phosphorus ylide, obtained from the independent synthesis of the corresponding phosphonium salts, with selected polyene-substituted aldehyde esters. Screening of the compds. was with one of two assays. One assay measured the ability of a retinoid to inhibit the phorbol ester induced increase of mouse epidermal ornithine decarboxylase (ODC) activity. The other assay measured retinoid-induced differentiation of the human myeloid leukemia cell line HL-60. In the ODC assay, all thirteen compds. were screened. The most active **heteroarotinoids** were ester I and the acid II. Both of these retinoids had ID50 values (dose required for half-maximal inhibition of phorbol ester induced ODC activity) of about 0.3 nmol. In comparison, the ID50 value for trans-retinoic acid III was 0.12 nmol while the ID50 values for acids IV and V were about 3.5 nmol. **Heteroarotinoids** VI and VII-XII had ID50 values of 35 nmol or greater. With a thiochroman unit, the most active acids in decreasing order of activity in the ODC assay were II > V > VI. Thus, simple replacement of the terminal propenyl system [C(16,17,18)] in IV with a cyclopropyl group produced acid VI with markedly reduced activity. With a **benzoic** acid group as part of the structure attached to the thiochroman unit, the ODC activity was enhanced as shown in I and II. The combination of the 2,2,4,4-tetramethylthiochroman group and the **benzoic** acid (or ester) terminal group seemed to enhance the biol. action which resembles that found with (E)-4-[2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-1-propenyl]**benzoic** acid, a well-known model system. Replacing the protons with fluorine in the C(12) Me group in the side chain and altering the orientation of the aryl groups around the double bond from anti to syn lowered ODC activity in both the thiochroman- and chroman-contg. systems. Esters VII and IX and acid VIII were essentially inactive while acid X exhibited a high ID50 in the ODC assay. In the chroman family, both ester XI and acid XII had unfavorable ID50 values. Since acid VIII differs only slightly from acid X [the latter is devoid of the geminal di-Me group at C(2)] and acid X differs only slightly from acid XII, possibly the nature of the heteroatom and the stereochem. at the .alpha. position may play important roles in regulating activity, but more examples are required to establish a trend. Changing the ring size from a fused six-six system to a five-six system led to ester Me (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl] **benzoate** (XIII) and acid (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thieny-5-yl)-1-propenyl]**benzoic** acid (XIV),

resp. In sep. expts. from those with of I-XII and known compds both XIII and XIV exhibited similar inhibition of ODC activity to that of III at the 34 nmol level. The ID50 values of XIV and XIV were, however, 10 and 200 times greater than that of III resp. In view of the toxicity of III, ester XIII may hold promise in chemotherapy. Of eight **heteroarotinoids** examd. in the HL-60 assay system, only acid IV displayed modest activity. This acid had an ED50 value (dose required for half-maximal effect) of 500 nM. In comparison, the ED50 for III was 50 nM. All of the other **heteroarotinoids** had ED50 values which were greater than 1000 nM.

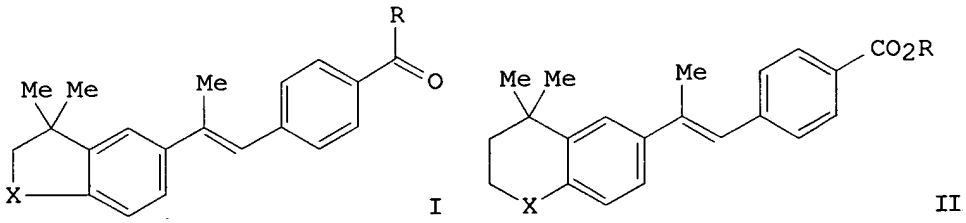
L13 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**: analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples
AN 1990:424286 CAPLUS
DN 113:24286
TI **Heteroarotinoids**: analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples
AU Gale, Jonathan B.; Rajadhyaksha, Shirish N.; Spruce, Lyle W.; Berlin, K. Darrell; Ji, Xinhua; Slagle, Andrew; Van der Helm, Dick
CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
SO Journal of Organic Chemistry (1990), 55(13), 3984-91
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 113:24286
AB A series of derivs. of E and Z isomers of 4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic** acid and 4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-1-propenyl] **benzoic** acid and sulfur-contg. counterparts were examd. in terms of 1H, 13C, and UV analyses for the purpose of establishing which parameters are diagnostic for identifying E and Z isomers in this family of **heteroarotinoids**. In addn., x-ray diffraction analyses for Me (E)-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-1-propenyl] **benzoate** (I), Me (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]**benzoate** (II), and Me (Z)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]**benzoate** (III) were performed to confirm the arrangement around the central double bond in the solid state in these rare examples contg. a fused, five-six-membered ring system. The proton NMR analyses of solns. of the E vs. the Z isomers, particularly the enhanced shielding of the vinylic proton and protons at "ortho" positions on the aryl groups attached to the double bond, provide markers to identify the Z isomers in these **heteroarotinoids**. In the 13C spectra, the Me C attached to the double bond was usually about 10 ppm downfield in the Z isomer compared to the counterpart in the E isomer. These data suggest that in soln. the two aryl rings in the Z isomers, (and possibly the E isomers, are turned out of the plane of the double bond, and, due to the closer proximity of the rings, induced shielding of nearby protons occurs to a greater extent in the Z isomers, compared to the E isomers. This evaluation is supported by UV spectral data which show max. in two ranges, namely at 210-270 and 280-350 nm. The "conjugation band" at the longer wavelength is always more intense, relative to the band at the shorter wavelength, in the E isomers. This implies improved overlap of p orbitals in the double bond with those in the aryl rings in the E isomers. In contrast, the band at shorter wavelength is more intense than the band at long wavelength in the Z isomers. These two features are clearly distinguishing for the two isomeric forms in soln. and relate to some degree to the stilbene isomerism. Characterization of I, II, and III via x-ray diffraction anal. of single crystals confirmed that the rings in both isomeric alkenes lack coplanarity with the central double bond in the solid state. The deviation from overall planarity is greatest for the Z

isomers with the internal torsional angle being 10./.degree. in III rather than the "ideal" value of 0.degree.. Moreover, the aryl rings are not far from being nearly perpendicular to each other in III. Mol. mechanics calcns., using the MMP2 program, indicate that the deviation from planarity is less than that found from x-ray anal. on solid III. These data provide a foundation for rapid identification of certain groups of **heteroarotinoids**. A comparison of crystal data of I and II with that of trans-retinoic acid was also made. The least-squares "fit" is quite satisfactory in spite of differences in conformational angles, and an RMS value of 0.90 .ANG. is calcd.

L13 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Heteroarotinoid compounds as anticancer agents
AN 1989:573986 CAPLUS
DN 111:173986
TI Heteroarotinoid compounds as anticancer agents
IN Berlin, Kenneth D.; Holt, Elizabeth M.; Ford, Warren T.; Thompson, Mark D.
PA Oklahoma State University, USA
SO U.S., 18 pp. Cont.-in-part of U.S. Ser. No. 598,482, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4826984	A	19890502	US 1987-9083	19870127
			US 1984-598482	19840409

OS CASREACT 111:173986; MARPAT 111:173986
GI



AB **Heteroarotinoids**, e.g., I (R = H, OH, OMe, OEt, etc.; X = S, SO, O), II (R = H, Me, Et; X = O, S, SO), etc., were prepd. as anticancer agents. Treatment of [1-(3,4-dihydro-4,4-dimethyl-2H-1-**benzothiopyran**-6-yl)ethyl]triphenylphosphonium bromide (prepn. given) with BuLi, followed by reaction with Et 4-formylbenzoate, gave, after workup, Et (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzothiopyran**-6-yl)-1-propenyl]**benzoate**. In the HL-60 cell differentiation assay, (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoate** exhibited an ED50 of > 3 .mu.M, vs. an ED50 of 200 nM for tetrahydrotetramethylnaphthalenylpropenylbenzoic acid.

L13 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**. Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells
AN 1987:576259 CAPLUS
DN 107:176259
TI **Heteroarotinoids**. Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the

induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells

AU Spruce, Lyle W.; Rajadhyaksha, Shirish N.; Berlin, K. Darrell; Gale, Jonathan B.; Miranda, Edgar T.; Ford, Warren T.; Blossey, Erich C.; Verma, A. K.; Hossain, M. B.; et al.

CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA

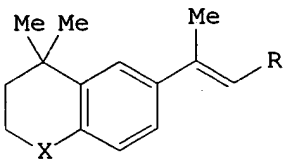
SO Journal of Medicinal Chemistry (1987), 30(8), 1474-82
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 107:176259

GI



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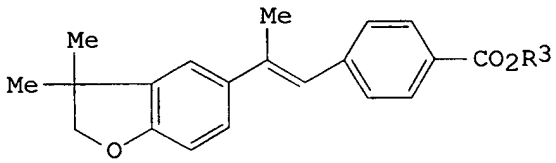


III

AB The heteroarotenoids I (X = S, R = CH:CHCMe:CHCO2R1, R1 = H, Et, 2-phthalimidoethyl) were prepd. from 6-acetyl-4,4-dimethylthiochroman. I (X = O, R = CH:CHCMe:CHCO2H) was similarly obtained from 6-acetyl-4,4-dimethylchroman (II). I (X = O, R = 4-R2C6H4, R2 = CO2Me, CH2OH, cyano, CHO) were also obtained from II. **Benzofurans** III (R3 = Me, H) were prepd. from 4-MeOC6H4Br and CH2:CMeCH2Cl. I (R = CH:CHCMe:CHCO2R1) showed high inhibition of ornithine decarboxylase, whereas I (R = 4-R2C6H4) and III were somewhat less active. In the HL-60 cell differentiation test I and III were substantially less active than trans-retinoic acid.

L13 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]**benzoate**

AN 1985:24869 CAPLUS

DN 102:24869

TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]**benzoate**

AU Waugh, Kristy M.; Berlin, K. Darrell; Ford, Warren T.; Holt, Elizabeth M.; Carrol, John P.; Schomber, Paul R.; Thompson, M. Daniel; Schiff, Leonard J.

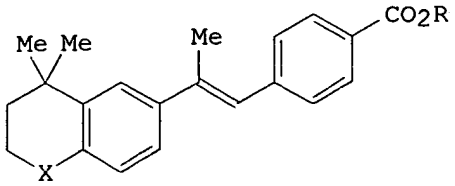
CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA

SO Journal of Medicinal Chemistry (1985), 28(1), 116-24
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

GI



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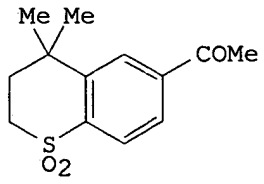

III

AB **Heteroarotinoids** I [X, R = S, Et (II); O, Et; S(O), Et; O, H] and the dioxide III were prepd. and evaluated for their vitamin A activity. X-ray anal. data for II and III are given.

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in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L15   STRUCTURE UPLOADED

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L15 HAS NO ANSWERS
L15   STR

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L19             0 SEA SSS SAM L18

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